Book of Abstracts

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“**According** to my calculations…” Computational and Theoretical Results

***Ab Initio* Composites to Quantum Dynamics: Challenges Across the Periodic Table**

Angela K. Wilson
Michigan State University, Department of Chemistry, East Lansing, Michigan, U.S.A.
akwilson@msu.edu

The prediction of thermodynamic and spectroscopic properties of transition metal species can be challenging due to increased molecular complexity, increased computational costs (i.e., computer time, memory, disk space), and more limited experimental data in comparison to early main group species. The challenges become even more substantial for the lanthanides and actinides. Strategies that are effective and ineffective in predicting thermochemical and spectroscopic properties, including approaches developed by our group, and applications that have provided insight about the lower part of the periodic table will be highlighted. As well, some of our recent work, which focuses on spin trapping processes will be overviewed.

ADSORPTION OF CR (VI) ONTO MICROPLASTICS: A MOLECULAR DYNAMICS SIMULATION STUDY

Abat Zhuldassov[1]

1 School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan, Kazakhstan.

E-mail: abat.zhuldassov@nu.edu.kz

Nowadays, microplastics (MPs) have become one of the emerging pollutants and many environmental organizations, including the WHO, are concerned with this oncoming threat to the different types of ecosystems and human health [1]. The problem is exacerbated by the fact that MPs, due to their sorption properties, can adsorb various toxic contaminants, including hexavalent chromium [2]. Cr (VI) adsorption on MPs represents a highly negative synergetic effect on the environment. For further risk evaluation and development of efficient and green technology for removing such combined toxic substances from various environments, fundamental research is necessary. Systematic studies of interaction mechanisms between MPs and contaminants will help us interpret the experimental results and predict various properties of the investigated system. Based on the above, the molecular dynamic (MD) method could be used as a potential tool for exploring Cr (VI) interactions with various types of MPs at the atomistic level. This work is dedicated to a comprehensive study of the adsorption energies and mechanisms in Cr (VI) – Polyethylene (PE), Cr (VI) – Polystyrene (PS), Cr (VI) – Polyvinylchloride (PVC) systems in the air, water, and vacuum environment using the MD approach.

In this work, classical force-field-based MD simulations were performed using the Forcite module from Material Studio 7.0 [3]. The polymer consistent forcefield (PCFF) was chosen for describing molecular dynamic interatomic interactions between chromium hexachloride chemical compound and polymers (PE, PS, PP). The degree of polymerization of each polymer's chain was 50, and the number of chains in a simulation was 10. All polymers prior to production run were equilibrated. 150 Å vacuum thickness was applied above each polymer. 1000 water molecules were used for water simulations, and eight N_2 and two O_2 were used for air simulation. NVT ensemble was applied for the production run. The temperature was controlled by the Nosé-Hoover thermostat. Electrostatic and Van der Waals energies were calculated by Ewald and Atom based summation methods, correspondingly, with the cutoff distance 15.5 Å. The time step was 1 fs, and the total simulation time was 1 ~ 10 ns. For each system, the periodic boundary condition was applied.

Our results showed that Cr (VI) adsorbed on all types of polymers in a vacuum and air medium. The order of intensity of adsorption energies between polymers and the metal ion in both cases goes as follows PVC-Cr (VI) > PS-Cr (VI) > PE-Cr (VI). The order correlates with the electronegativity and partial negative charges of atoms present on PVC, PS, and PE (Cl > sp^2 C > sp^3 C). It was observed that the adsorption process of ions in PVC and PS occurred through the electrostatic and van der Waals (vdW) forces, while in PE only through the vdW. In an aqueous environment, our simulations did not show Cr (VI) adsorption on polymers, which could be attributed to the formation of a hydration shell around chromium (VI) chloride. Also, it was found that Cr (VI) on adsorbed state inside the polymer matrix can desorb and release into the aqueous phase.

It can be concluded that the Cr (VI) adsorbs on MPs in a vacuum and air environment, while in water it remains unabsorbed. The strength of adsorption energy depends on the chemical properties of an atom present on polymer. Adsorption process in PVC and PS occurred through both forces electrostatic and vdW, while in PE only through the vdW forces. Cr (VI) tends to desorb from the polymer matrix and release into the aqueous phase.

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COMPUTATIONAL PHOTOCHEMISTRY IN ACTION: CHARGES, CROSSINGS AND CONTROL

Michael J. Bearpark[1]

[1]Department of Chemistry, Imperial College London, Molecular Sciences Research Hub, 82 Wood Lane, W12 0BZ, London, UK

Photoionisation can create a coherent superposition of electronic states and therefore initiate electronic dynamics in atoms and molecules. Observing and controlling such dynamics experimentally is a target of spectroscopy on the attosecond timescale, supported by computation.

Theoretical studies of pure electron dynamics at fixed nuclear geometries have demonstrated oscillatory charge migration. Using a CASSCF implementation of the Ehrenfest method, we can study the evolution of a non-stationary electronic wavefunction, both for fixed atomic nuclei and where the nuclei are allowed to move. For benzene cation, with nuclei fixed, there is no electron dynamics in this case. However, if we add substituents that break symmetry but do not radically alter the electronic structure, we see charge migration: oscillations in the spin density that we can correlate with particular localised electronic structures, with a period depending on the energy gap between the states initially populated. The coupling to nuclear motion is substituent dependent, although the effect of sampling the ground state nuclear wave packet appears to mask any coherences that survive in this case.

We systematically investigated the effect of changing the relative amplitudes and phases in the initial superposition of electronic states. By controlling the initial electronic conditions in this way, we can begin to control the subsequent nuclear motion, and this is currently an active area of research.

DEMYSTIFYING THE ROLE OF STEAM INJECTION IN RETARDING THE METAL LOSS DURING SYNGAS/FE INTERFACIAL REACTIONS

El Tayeb Bentria[1], Salawu Omotayo Akande[2], Abitha Ramesh [3], Nicholas Laycock [3], Wouter Hamer [4], Normand Mousseau[5], Charlotte S. Becquart[6], Othmane Bouhali[2] and Fedwa El-Mellouhi[1]

[1] Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. BOX 34110,Doha,Qatar
[2]Texas A&M University at Qatar, P.O. Box 23874, Doha, Qatar
[3] Qatar Shell Technology Center, QSTP, Doha, Qatar

[4] Shell Technology Centre Amsterdam, Netherlands

[5] Département de physique and Regroupement québécois sur les matériaux de pointe, Université de Montréal, Montréal (QC) Canada H3C 3J7.

[6] Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

E-mail: felmellouhi@hbku.edu.qa (F.E), ebentria@hbku.edu.qa (E.B)

Atomistic simulation methods such as molecular dynamics are powerful tools for exploring, developing, and optimizing the properties of materials. Reactive force field “ReaxFF” potentials are best suited for simulating the interfacial catalytic reaction of hydrocarbons on metal surfaces. However, ReaxFF with its current formalism hardly captures concurrently the broad range of reactions, such as the kinetics of CO adsorption, dissociation, atomic carbon diffusion in iron systems and metal self-diffusion [1]. This poses challenges for the currently available potentials to account for the various processes leading to metal loss for example. We overcome this limitation by extending the standard parameter setup to allow specific adaptation to the interactions of carbon at the surface and in the bulk separately. After testing the new potential, we show that this developed “Extended” reactive force field potential enables us to account for the effect of steam on mitigating metal loss corrosion. We built an iron system containing multiple grain boundaries consisting of more than 5000 atoms exposed to syngas mixture at 773 K. Our simulations demonstrate that the presence of water on a clean Fe surface promotes different catalytic reactions at the beginning of the simulations that boost the C, H, O diffusion into the sample. At later stage, the formation of oxide scale leads to an elevated concentration of H_2O/OH molecules on the surface due to the decrease in Fe affinity to dissociated water. The developed analysis is expandable to other syngas mixtures and simulations conditions of interest where metal loss might be observed [2].

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HYDROGEN EVOLUTION CATALYSED BY METAL-DECORATED DEFECTED GRAPHENE AND HEXAGONAL BORON-NITRIDE

Dušan N. Sredojević,[1,2] Milivoj R. Belić,[1] Edward N. Brothers,[1] and Željko Šljivančanin[2]

[1]Texas A&M University at Qatar, P.O.Box 23874 Doha, Qatar
[2]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O.Box 522, RS-11001 Belgrade, Serbia

E-mail: dusan.sredojevic@qatar.tamu.edu

We used DFT calculations in the study of atomic hydrogen adsorption and recombination over various single-atom catalysts, modeled by embedding nine different transition metals into the three types of monovacancies of graphene and *h*-BN. [1] In this way, we selected several candidates for the SACs that might be able to catalyze hydrogen evolution reactions with efficacy comparable to that of the platinum surface. We found that Ru, Os, and Co adatoms at the nitrogen-vacancy of the *h*-BN (V_N) provide a suitable environment for the H adsorption, with diminishing free energy of the adsorption of two H atoms at Ru@V_N. The small values of adsorption free energy were calculated for Os@V_N, Pd@V_B, and Co@V_N, which are -0.02 eV, 0.08, and -0.13 eV, respectively. The nearly free energy neutral H adsorption is accompanied with very favorable kinetics of the H_2 recombination. The calculated activation energies at Os@V_C, Os@V_N, and Co@V_N are as low as 0.04, 0.11, and 0.16 eV, respectively, that would enable fast H_2 recombination at room temperatures.

Since the Earth's crust is much richer in Co than in platinum, in terms of the cost, this metal could be a valuable alternative to catalyze HER. On the other side, Ru is more scarce and yet cheaper than platinum, and Os is one of the rarest metals in Earth's crust. Thus, from the economic point of view, the search for the efficient catalyst for HER, based on single metal atoms embedded into monovacancy sites of graphene and *h*-BN, should be focused on Co and Ru-decorated *h*-BN.

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IMPROVED METHANE C-H ACTIVATION COMPLEXES BASED ON $N[2\text{-}P^iPr_2\text{-}4\text{-methylphenyl}]^{2-}Ti{=}CH^tBu(CH_2{}^tBu)$

Dragan B Ninković,[1] **Salvador Moncho**,[1] **Snežana D. Zarić**,[2] **Michael B. Hall**,[3] **Edward N. Brothers**[1]

[1]*Chemistry Department, Texas A&M University at Qatar, Doha, Qatar*
[2]*Department of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, Serbia*
[3]*Chemistry Department, Texas A&M University, College Station, TX 77843*
E-mail: dragan.ninkovic@qatar.tamu.edu

The inertness of the carbon-hydrogen bond (C-H) is the main reason why converting natural gas to added-value chemicals is a challenging process. An ideal transition-metal catalyst for C-H bond activation, practical at low temperatures and with good selectivity, is still elusive despite 50 years of work in this field. We investigated (PNP)Ti=CHtBu(CH2tBu), where PNP=N[2-PiPr2-4-methylphenyl]2- complex that activates C-H bonds by 1,2- addition reaction processes, The transient titanium alkylidyne complex can activate both sp2 and sp3 C-H bonds under mild conditions [1-3]. Mayor advantage of this complex is that titanium is less expensive than other transition metals commonly used in catalysis, and this complex does not require photochemical activation.

We investigated a series of complexes based on a titanium complex capable of activating C-H bonds under mild conditions. In addition to the activation of methane, a following reaction of tautomerization to a terminal methylidene is also explored, because of its synthetical interest. Analogous complexes with other transition metals such as scandium, titanium, vanadium, and chromium. Both isoelectronic (with the same number of electrons in the metal) and isocharged (with the same charge and oxidation state of the metal) complexes, were checked. In addition to the original PNP ligand, some of the most promising ligands from previous work were tested [4]. Vanadium complexes are promising for methane C-H activation due to the lower barrier, particularly V(V). Scandium high barriers prevents its use in this reaction while chromium overstabilizes strongly the alkylidine intermediate, potentially stopping the reaction. The effect of the ligands is confirmed to be qualitatively transferable from the Ti reference to other metals, but they have weaker effects on the activity of the system.

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Machine Learning from Large and Sparse Data for Novel materials discovery

Fadwa El Mellouhi[1]

[1]Qatar Environment and energy Research Institute, Hamad Bin Khalifa University,
Doha, Qatar

Materials discovery has prospects of significant acceleration in the upcoming years thanks to the adaptation of data-science and machine learning techniques. In this talk, I will give an overview of the latest advances in this field with focus on materials for energy and environmental applications. I will show how large and sparce datasets constructed from density functional theory (DFT) calculations [1] or experiments [2] can be used to perform a systematic analysis of structure-to-property relationships. Focusing on the correlations between the structural deformations and the thermodynamic stability of compounds, various machine learning algorithms were trained then tested[1,2]. I will also highlight how our approach offers an interesting guideline on how to engineer novel materials compositions enabling to reduce the huge space of experimental trial and error.

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MAKING THE INACCESSIBLE, ACCESSIBLE: NOVEL TECHNIQUES FOR OBTAINING ACCURAGE QM/MM FREE ENERGIES AT AFFORDABLE COSTS

Lee Woodcock[1]

[1]Department of Chemistry, University of South Florida, Tampa, FL 33620

hlw@mail.usf.edu

Indirect (S)QM/MM free energy simulations (FES) are vital to efficiently incorporating sufficient sampling and accurate (QM) energetic evaluations when estimating free energies of practical/experimental interest. Connecting between levels of theory, i.e., calculating ΔA(low→high), remains the most challenging step within an (S)QM/MM indirect FES protocol. To improve calculations of ΔA(low→high), we must: (1) compare the performance of all FES methods currently available; and (2) compile and maintain datasets of ΔA(low→high) calculated for a wide variety of molecules so that future practitioners may replicate or improve upon the current state-of-the-art. Towards this end, we have carried out several benchmark studies, based on a recently introduced "HiPen" dataset, which seek to optimize the convergence of ΔA(low→high). These studies focus on (1) optimizing protocols for carrying out non-equilibrium work simulations in combination with Jarzynski's equation to ensure both robustness and efficiency, and (2) evaluating our recently developed machine learning-based force matching technique to assist in bridging the gap in, often, disparate levels of theory. Progress in both of these directions will be reported in this presentation.

NONEQUILIBRIUM GREEN'S FUNCTIONAL FORMALISM FOR PREDICTIVE MODELLING IN NANO- AND MOLECULAR ELECTRONICS

Golibjon R. Berdiyorov and Hicham Hamoudi

Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha, Qatar
E-mail: gberdiyorov@hbku.edu.qa

Nonequilibrium Green's functional formalism is known to be an effective method in studying electronic transport at the nanoscale [1]. Based on defining the Green function (i.e. a function of two spacetime coordinates), this approach allows one to calculate the time-dependent expectation parameters such as currents and charrier densities, electron injection and removal energies and the total energy of complex system.

In this work, we use nonequilibrium Green's functional formalism in combination with density functional theory to make predictive modelling for the following systems to explore their potential for practical applications in nanoelectronics and molecular electronics:

- **Carbon nanotube (CNT)–metal junctions as nanoscale diodes**. We show that the rectification properties of the system can be enhanced dramatically by chemical doping (e.g. fluorination) of the tip of CNTs, originating from voltage-dependent charge localization in the system [2].
- **Graphene-based geometry diodes**. We show the possibility of creating geometry diodes through spatial fluorination of monolayer graphene. This system exhibits enhanced diode properties (i.e, larger current rectification and smaller differential resistance) as compared to the system, where the asymmetry is created by direct structural nano-patterning [3].
- **Metal-insulator-metal diodes**. The main goal of this work was to study the effect of insulator thickness on the electronic transport properties of metal-insulator-metal diodes. We show that the current rectification and nonlinearity increase linearly with the layer thickness, whereas the differential resistance increases exponentially with increasing the thickness [4].
- **Molecular junctions with permanent dipole moment**. Such molecular junctions show clear current rectification due to polar nature of the molecules. In addition, the presence of the permanent dipole enhances the current through the junction for both polarities of the applied voltage [5].
- **Molecular junctions with functional edge groups**. We study the electronic transport properties of biphenyl and phenyl-pyridine molecules asymmetrically anchored to gold electrodes via different edge groups. We show that the diode properties of such molecular junctions can be greatly enhanced by tuning the edge groups [6].
- **Multipodal molecular junctions (diazatriptycene molecule)**. Such molecules are promising for creating defect free and densely packed molecular self-assemblies. We show that due to its structural asymmetry, the molecule shows a clear current rectification, where the level of the rectification depends on the nature of the head group [7].

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Revisiting the Double-Link Atom Approach

Michael R. Jones and Bernard R. Brooks

Laboratory of Computational Biology, National Heart, Lung, and Blood Institute, National Institutes of Health, Bethesda, MD, 20814
Mjones@chemistry.msu.edu

Accurate modeling chemical reactions in condensed phases with combined quantum mechanical and molecular mechanical (QM/MM) can be a challenge. In this work, QM/MM methods employing different link atom schemes and fragment caps are carried on small molecules and tripeptides in order to determine optimal parameters for accurately predicting physical properties of more complex systems.

SELECTIVE C-H OXIDATION OF ETHYLBENZENE TO ACETOPHENONE USING COBALT PHOSPHINE OXIDE COMPLEXES

Salvador Moncho,[1] *Chi Chen,*[2] *Stafford W. Sheehan,*[2,]* *Edward N. Brothers*[1,]*

[1] Science Program, Texas A&M University at Qatar, PO Box 23874, Education City, Doha, Qatar

[2] Catalytic Innovations, 151 Martine Street, Fall River, MA 02723, USA

*Correspondence: edward.brothers@qatar.tamu.edu (E.N.B.), staff@catalytic-innovation.com (S.W.S.)

Selective oxidation of C-H bonds is required for reactions ubiquitous in chemical industry, and understanding the mechanisms of these reactions will accelerate development of the next generation of catalysts. Highly selective homogeneous cobalt catalysts bearing phosphine oxide ligands are synthesized to support mechanistic studies that investigate what drives selectivity in ethylbenzene oxidation, as a model reaction. Computational studies considered three mechanisms: (1) an external outer-sphere reaction wherein the metal's primary role is facilitating radical formation, (2) inner-sphere coordination of the substrate combined with outer-sphere radical formation in a semi-external pathway, and (3) a fully inner-sphere reaction where oxidation is carried out by an attack from a Lewis base. Experimental and computational kinetic modeling together with byproduct analysis suggests that the reaction proceeds with highest activity and selectivity for the methyl ketone product by the second pathway. By elucidating this reaction mechanism, we show how both inner-sphere and outer-sphere coordination must be controlled to achieve high selectivity in C-H oxidation catalysis.

THE STABILITY OF THE MONOETHANOLAMINE-CO2 ZWITTERION AT THE VAPOUR/LIQUID WATER INTERFACE: IMPLICATIONS FOR LOW PARTIAL PRESSURE CARBON CAPTURE.

Alessandro Sinopoli[1], Ahmed Abotaleb[1], Fabio Pietrucci[2], and **Ivan Gladich**,[1, *]

[1]Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. Box 34410, Doha, Qatar

[2]Sorbonne Université, Muséum National d'Histoire Naturelle, UMR CNRS 7590, IMPMC, F-75005 Paris, France

[*]**Electronic mail:** igladich@hbku.edu.qa

Control CO_2 conversion in aqueous amine solutions is impelling for the development of cost-effective industrial technologies for carbon conversion into added-value products, as well as for the design of near-future devices for direct air capture working at low (e.g., ambient) partial pressure. Here, we have determined the stability of CO_2-monoethanolamine zwitterion and its chemical conversion to carbamate at the vapour/liquid water interface by *first-principles* molecular dynamics coupled with a recently introduced enhanced sampling technique. Contrary to the bulk water case, our results show that both the zwitterion and carbamate ions are poorly stable at the vapour/amine aqueous interface, further stating the differences between the homogeneous and heterogeneous CO_2 chemical conversion. This work states the potential of novel atomistic simulation approaches in enabling the design of capture systems working at low (e.g., ambient) CO_2 partial pressure that may overcome the limits of the current absorbants, as well as in addressing the well-known and energy-consuming problem of amine regeneration from scrubbing solution.

Advanced Functional & Emerging Materials

Bridging the gap between homogenous and heterogeneous catalysis: Solubilizing MOFs for In Situ IR-SEC study for electrocatalytic CO_2 reduction

Muhammad Sohail, Sherzod T. Madrahimov and Ashfaq A. Bengali

Texas A&M University at Qatar, Science Department, Texas A&M Engineering Building,
Education City, P. O. Box 23874, Doha, Qatar

Email: muhammad.sohail@qatar.tamu.edu

Metal-organic frameworks (MOFs) are known to be excellent heterogeneous supports for their regular crystalline structures, tunable porosity, and controllable particle size with a variety of topologies [1]. The diversity of integrated functional organic moiety in the MOFs provides facile opportunities to covalently attach a molecular catalyst at a well-defined position to explore the catalytic mechanisms by which they operate. Taking advantage of the functional moiety, recently, molecular catalysts have been grafted onto MOFs for different applications such as CO_2 reduction [1]. In this work, heterogeneous MOF support is solubilized along with a grafted molecular catalyst to obtain mechanistic information by identifying key intermediates and their temporal profile, figure 1 [2]. IR spectroelectrochemistry (IR-SEC) technique is being used, which allow in situ reaction intermediates monitoring in electrocatalytic processes [3].

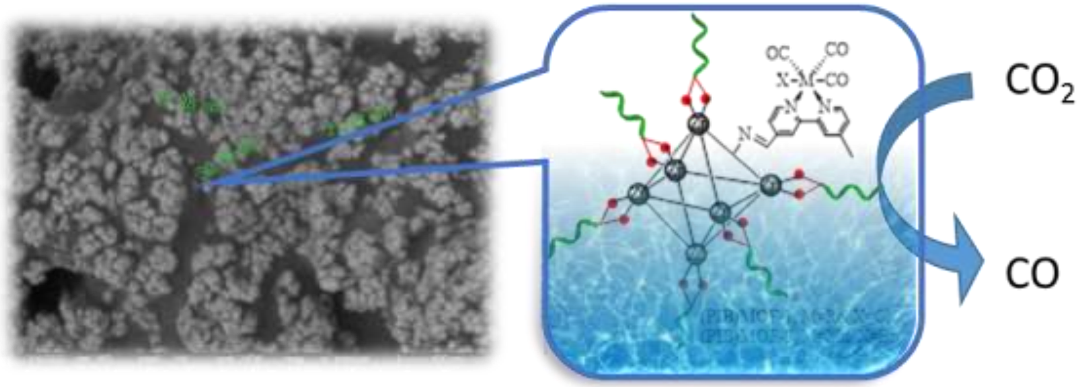

Figure 1. Solubilized catalyst immobilized MOF nanoparticles for in situ IR-SEC study.

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Catalytic reduction of N_2O in the presence of methane over Cu-Fe oxide thin-film catalysts

Muhammad Waqas[1,2,*], Achraf El Kasmi[1,3], Syed Murawat Abbas Naqvi[4], Muhammad Ammar[5]

[1] Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing 100190, China.
[2] Department of Mechanical Engineering, College of Engineering and Technology, University of Sargodha, Sargodha, Pakistan.
[3] Laboratory LSIA, UAE/U02ENSAH, National School of Applied Sciences of Al Hoceima, Abdelmalek Essaadi University, Al Hoceima 32003, Morocco.
[5] Department of Mechanical Engineering, NFC Institute of Engineering and Fertilizer Research, Faisalabad 38000, Pakistan.
[5] Department of Chemical Engineering Technology, Government College University, Faisalabad 38000, Pakistan.
* Corresponding author email: waqas.muhammad@uos.edu.pk

Abstract: A series of $CuFeO_x$ thin-film catalysts were prepared with different Fe contents using a one-step method as well as tested for the catalytic reduction of N_2O (nitrous oxide) in the presence of CH_4 at a high GHSV of 185,000 mL g^{-1} h^{-1}. Thin-film catalysts are recently recognized as promised catalysts due to their reduced amount of materials and good catalytic activity, leading to low efficiency-cost catalysts. With the increase of iron, it strongly affects the dispersion and leads to the creation of a less-active segregated Fe_2O_3 phase, which was confirmed by XRD, EDX, and XPS outcomes. The results show that the synergistic properties between Cu and Fe, which affect the $CuFeO_x$ film catalysts in many aspects, such as the hollows-like texture, specific surface area, nano-crystallite size, the surface contents of Cu^+, Fe^{3+} and oxygen species, the reductive strength and the strong active sites on the surface The strategy adopted here to tailor the activity through low doping Fe-oxide catalysts could establish a promising way to improve the catalytic reduction of N_2O with CH_4.

Keywords: Catalytic reduction; Thin-film catalysts; Doping strategy; Density functional theory calculations; N_2O decomposition.

Computational Catalysis for Sustainable Future: An Industrial Perspective

Sharankumar Shetty

Shell Technology Centre-Bangalore

Sharankumar.shetty@shell.com

Growing demand on the utilization of fossil-based feedstock has raised serious environmental concerns and requires a significant overhaul of new technologies to decarbonize our economies for a sustainable society. In recent years, computational approaches in conjunction with high performance computing has made an incredible progress to accelerate the experimental research to achieve their goals towards greener chemical processes.

In this presentation, we will discuss the role of computational methods to characterize the underlying catalytic reactions that will help to design new generation catalysts for sustainable processes. We will focus on the topics such as CO2 capture and conversion, sustainable chemicals and Fischer-Tropsch process.

CORROSION PROTECTION OF STEEL THROUGH Ni-P-B_4C NANOCOMPOSITE COATING FOR OIL AND GAS INDUSTRY.

Osama Fayyaz[1],Izza Fathima[2], Fatima Aziz[2], Sara Bagherifard[4], M. F. Montemor[3], R. A. Shakoor[1*]

[1]Center for Advanced Materials (CAM), Qatar University, 2713, Doha, Qatar.

[2]Department of Chemical Engineering, Qatar University, Doha Qatar

[3]Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Portugal

[4]Department of Mechanical Engineering, Politecnico di Milano, Milan, Italy

*E-mail:*shakoor@qu.edu.qa

Improved mechanical properties and enhanced corrosion resistance are among the major requirements for decreasing operational cost in steel-based industries. Nickel-phosphorus coatings are reported to possess better corrosion resistance along with inadequate mechanical strength. Boron carbide nanoparticles are well known refractory material for their hardness and inertness. In this study, reinforcement and increase of B_4C was investigated based on compositional, microstructural, mechanical and electrochemical properties of as prepared nanocomposite coatings. Modified Watts bath was employed to carry out conventional electrodeposition for developing nanocomposite coating. XRD spectra demonstrates the nanocrystalline nature of the coatings, XPS results confirms the successful deposition of boron carbide nanospecies and chemical states of other elements. SEM micrograph reveals the microstructural grain-refinement with increase in concentration of B4C nanoparticles. Nanoindentation profile and microhardness result confirms the enhancement in mechanical properties which can be elucidated to combination of Hall-Petch effect and formation of composite structure. EIS and Tafel plots show the improvement in corrosion resistance as a result of minimizing the penetration of corrosive species by protecting active area. Ni-P-B_4C nanocomposite coatings offer an exciting option for their application in electronics, automotive, aerospace, oil, and gas industries.

CRYSTAL STRUCTURE AND OPTICAL PROPERTIES OF PEROVSKITES $Sr_3Fe_{2+x}Mo_{1-x}O_{9-3x/2}$ (0.3 ≤x≤ 1)

A. El Hachmi,[1] **B. Manoun,**[1,2] **M. Sajieddine,**[3] **Y. Tamraoui,**[2] **S. El Ouahbi**[4]

[1] *Chemistry Department, University Hassan 1st, Faculty of Sciences and Techniques, Settat, Morocco*
[2] *Materials Science and Nano-engineering (MSN), University Mohammed VI Polytechnic, Ben Guerir, Morocco*
[3] *Material Physics Laboratory, Faculty of Sciences and Techniques, Sultan Moulay Sliman University, Beni-Mellal, Morocco*
[4] *LPMMAT, Faculty of Sciences - Ain Chock, University Hassan II, Casablanca, Morocco*
E-mail: elhachmi.abdelhadi@gmail.com

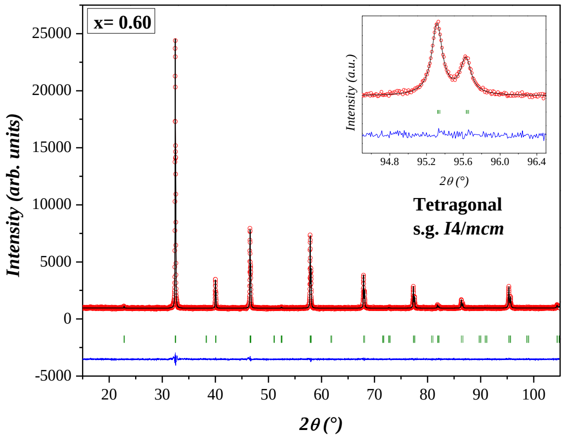
Abstract

Perovskites-type oxides $Sr_3Fe_{2+x}Mo_{1-x}O_{9-3x/2}$ (x= 0.30, 0.45, 0.60, 0.75, and 1.00) were synthesized in polycrystalline form using solid-state reaction, in air. These oxides have been studied at room temperature using of XRD, Mössbauer and UV-vis spectrophotometry.

The crystal structures were refined by Rietveld's method, and revealed that this series adopts two phase transitions from a tetragonal *I*4/*mcm* (x= 0.30, 0.45, and 0.60) to a simple cubic *Pm*3*m* (x= 0.75) to another tetragonal *P*4/*mmm* (x= 1.00) phase.

The values of the isomer shift (IS) and quadrupole splitting (QS) confirm that the formal oxidation state of iron containing our compounds consist of the mixed valence of the Fe^{3+} and Fe^{4+} cations for octahedral environment. The Mössbauer spectrum of the sample (x= 0.75) - $SrFe_{0.917}Mo_{0.083}O_{3-\delta}$ is consistent with Fe in a cubic lattice site. The direct bandgap energy increases from 1.70 to 2.25 eV with increasing x.

Spectral dependence of optical parameters such as; absorption coefficient, refractive index, extinction coefficient, optical conductivity, real and imaginary parts of the complex dielectric function, complex electric modulus and complex impedance were performed in the range 1.54 - 4.94 eV using UV- spectroscopy experiments.



DESIGN STRATEGIES TO SYNTHESIZE POLYMER NETWORKS FOR GAS ADSORPTION AND ENVIRONMENTAL REMEDIATION APPLICATIONS

Noorullah Baig, Suchetha Shetty, Bassam Alameddine,
Gulf University for Science and Technology, West Mishref, Kuwait
email: alameddine.b@gust.edu.kw

New design strategies are disclosed to prepare conjugated microporous polymers (CMPs) using versatile metal-catalyzed [3+2] cyclopentannulation and [4+2] cyclobenzannulation reactions. The resulting polymers[1-2] display high solubility and excellent chemical stability, which allow for their structural and photophysical characterization by various instrumental analysis techniques such as, gel permeation chromatography (GPC), 1H- and 13C-nuclear magnetic resonance (NMR), Fourier transform infrared (FTIR), UV-vis absorption, and emission spectroscopies. GPC chromatograms display a high relative weight-average (Mw) molecular weight in the range of 15.8 to 41 KDa with a polydispersity index (Đ=Mw/Mn) ranging from ~2-4. The intrinsic microporosity properties were investigated using nitrogen adsorption measurements, revealing Brunauer-Emmett-Teller (BET) surface areas up to 794 m^2g^{-1} and average pore volumes reaching 0.63 cm^3g^{-1}. Inspection of the adsorption properties of the resulting target polymers divulges their high iodine uptake with a maximum of 200 wt%. Moreover, some copolymers divulge their efficiency as selective dye adsorbents by their quantitative adsorbtion of methylene blue over methyl orange from aqueous solution.

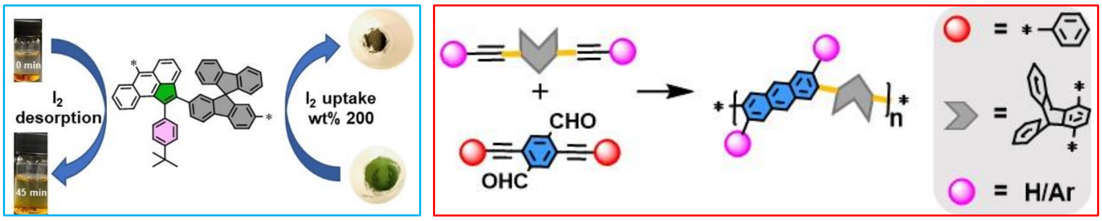


Fig. 1 Cyclopentannulation (left) and cyclobenzannulation (right) polymerization reactions

1. Baig, N.; Shetty, S.; Al-Mousawi, S.; Alameddine, B., Synthesis of Conjugated Polymers via Cyclopentannulation Reaction: Promising Materials for Iodine Adsorption. *Polymer Chemistry* **2020,** *11* (17), 3066 - 3074.

2. Baig, N.; Shetty, S.; Al-Mousawi, S.; Alameddine, B., Conjugated microporous polymers using a copper-catalyzed [4 + 2] cyclobenzannulation reaction: promising materials for iodine and dye adsorption. *Polymer Chemistry* **2021,** *12*, 2282 - 2292.

DESIGNING HIGH PERFORMANCE ORGANIC SEMICONDUCTING POLYMERS

Iain McCulloch

Department of Chemistry, University of Oxford, Oxford, OX13TA, UK

Understanding the impact of both the organic semiconducting polymer design and processing conditions, on both molecular conformation and thin film microstructure has been demonstrated to be essential in achieving the required optical and electrical properties to enable a range of devices. Synthesis of conjugated aromatic polymers typically involves carbon coupling polymerisations utilising transition metal catalysts and metal containing monomers. This polymerisation chemistry creates polymers where the aromatic repeat units are linked by single carbon-carbon bonds along the backbone. One consequence of this single bond link is that the aromatic repeat units have the freedom to twist with respect to each other, introducing energetic disorder. We present design and synthesis strategies to restrict or even eliminate this tortional disorder through enhancement of non-covalent interactions. Additionally, an aldol condensation reaction was explored, in which a bisisatin monomer reacts with a bisoxindole monomer to create an isoindigo repeat unit that is fully fused along the polymer backbone. This aldol polymerization requires neither metal containing monomers or transition-metal catalysts, opening up new synthetic possibilities for conjugated aromatic polymer design, particularly where both monomers are electron deficient. Polymers with very large electron affinities can be synthesised by this method, resulting in air stable electron transport, demonstrated in solution processed organic thin film transistors. We present an electrical, optical and morphology characterisation of polymer thin films, illustrating structure-property relationships for this new class of polymers.

Detection of hazardous gases using lead halide perovskite nanoparticles

Ahmad I. Ayesh[a], S.A. Alghamdi[b], Belal Salah[a], S.H. Bennett[b], C. Crean[b], P.J. Sellin[b]

[a] Physics Program, Department of Math., Stat. and Physics, College of Arts and Sciences, Qatar University, P.O.Box 2713, Doha, Qatar
[b] Department of Physics, University of Surrey, Guildford GU2 7XH, UK

Abstract

We report the fabrication and testing of a highly sensitive gas sensor based on perovskite nanoparticles. The nanoparticles were synthesized from the metal halide perovskite formamidinium lead bromide ($FAPbBr_3$) using a relatively simple solution-growth method. The morphology, photoconductivity, and electrical characteristics were examined for the produced nanoparticles. The nanoparticles were used to fabricate conductometric gas sensors that found to exhibit high sensitivity and selective to H_2S gas in the form of changes in the electrical conductivity. The response of the sensor to H_2S gas reveled a high sensitivity to gas concentrations within the range 0.5 – 100ppm, with a reasonably fast response time of below one minute under ambient room conditions.

Keywords

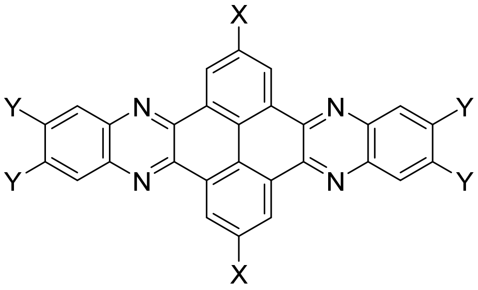
$FAPbBr_3$; perovskite; gas sensor; H_2S

DISCOTIC LIQUID CRYSTALS: FROM QUINOXALINOPHENANTHROPHENAZINE TO ISOINDIGO DISCOTICS

Bilal R. Kaafarani[1]

[1]Department of Chemistry, American University of Beirut, Beirut 1107-2020, Lebanon
Email: bilal.kaafarani@aub.edu.lb

Discotic Liquid Crystals (DLCs) are generally formed of a discoid core to which extended flexible chains are attached. DLCs have been exploited in a wide range of electronic applications particularly in organic photovoltaics (OPVs) and Organic Field-Effect Transistors (OFETs). Fused, ladder-type organic materials have inherent advantages, such as extended π-frameworks, favorable stacking behavior in the solid state, conductivity, and high field-effect mobility. The planarity of the cores facilitates the efficient cofacial stacking of these materials in the solid state and increases the intermolecular π-orbital overlap leading to their self-assembly into π-π columnar stacks. In this talk, we will cover our research journey working on DLCs starting with the quinoxalinophenanthrophenazine core **1** to the isoindigo core **2**. We will also discuss the different optical properties and features of these compounds.



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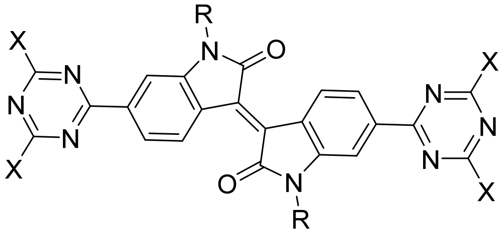
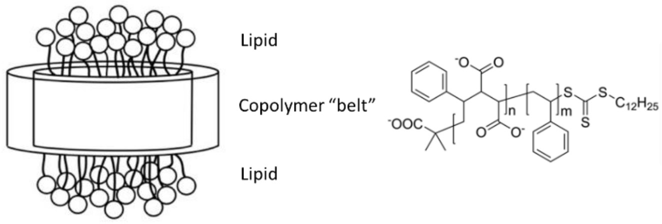


2

FUNCTIONAL STYRENE MALEIC ACID COPOLYMERS FOR MEMBRANE PROTEIN STUDIES IN LIPID NANODISCS

George M. Neville[1], Karen J. Edler[1], Aya A. Nasser[2] and Gareth J. Price[1,2]
[1] Department of Chemistry, University of Bath, Bath, United Kingdom
[2] Department of Chemistry, Khalifa University, Abu Dhabi, United Arab Emirates
E-mail: gareth.price@ku.ac.ae

The proteins located in biological cell membranes are hugely important in a wide range of processes and are the target of many pharmaceutical and therapeutic interventions [1]. However, their study is complicated since their structure and function depend on the surrounding lipids. Most methods of extracting MPs result in denaturing or other structure modifications. A recent development that overcomes these problems is the discovery of ‘styrene maleic acid lipid particles’, SMALPs [2]. These form when the poly(styrene-co-maleic acid) copolymer ‘wraps’ around the lipid bilayer to form ‘nanodisks’ which are 10 – 30 nm in diameter and can maintain encapsulated protein in their native state. The action of the copolymers depends on the delicate balance between its hydrophobic and hydrophilic regions. A number of different polymers have been developed but SMA. remains the most widely used. However, questions remain as to the precise mechanism of action and the optimum polymer structure.



Commercial variants of SMA are produced by radical polymerization and so have high polydispersity. In order to study SMALP formation, copolymers with a narrow distribution of chain have been produced by RAFT polymerization. In addition to the narrow polydispersity, these materials have a block of alternating SMA with a styrene homopolymer tail. Here we report the preparation of a range of molecular weights and the rate at which lipid SMALPs are formed has been measured by turbidimetry. Preliminary results suggest that the copolymer chain length has only a small influence on the process. However, structural differences between the RAFT copolymer and a commercial SMA2000 had a larger difference.

In related work [3], fluorescently-labelled variants of poly(styrene-co-maleic acid), SMA, have been synthesised through inclusion of low ratios of vinyl anthracene or pyrenemethyl acrylate into the RAFT reaction. This had negligible effect on nanodisc formation upon interaction with lipids. In contrast with side chain modification of commercial materials, by incorporating fluorophores directly in the polymerisation feed, the extent of functionalisation may be feasibly controlled and more effective copolymers rationally designed.

Here, Förster resonance energy transfer (FRET) has been used to probe the proximity between the model protein gramicidin and the copolymer annulus, indicative of interactions which may threaten the native functioning of MPs in these systems. Also potentially useful in elucidating nanodisc self-assembly, the copolymers presented aggregation-caused-quenching. This was utilised to monitor the transition from aggregated polymer to nanodisc annulus over time. The work reported here lays the foundation to exploit the synthetic control afforded by RAFT to precisely label specific components of the copolymer structure, allowing the mechanism of SMALP formation to be examined in detail.

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High Performance Asymmetric Supercapacitors Based on Mo-doped ZnO nanoflakes on Ni-foam

Awais Ali [1,2], Iqra Hameed [3], Muhammad Ammar [1,4*]

[1]*Department of Chemical Engineering Technology, Government College University, Faisalabad 38000, Pakistan.*

[2]*Department of Chemical Engineering, NFC Institute of Engineering and Fertilizer Research, Faisalabad 38000, Pakistan.*

[3]*Department of Electrical Engineering, FAST-National University of Computer & Emerging Sciences, Chiniot-Faisalabad 38000, Pakistan.*

[4]*University of Chinese Academy of Sciences, Beijing, 100049, China.*

Email Corresponding Author: mammar@gcuf.edu.pk (M. Ammar), Tel/Fax: +92-41-9203027

Nanoflakes of Mo-doped ZnO is grown on Ni foam (NF) using a single stage hydrothermal reaction. Excellent dimensional stability and structural features, less contact resistance because of direct growth, and high electrical conductivity due to synergetic effects have made it a perfect candidate for electrode material. Mo-doped ZnO show superior specific capacitance of 2296 F g^{-1} at 1 A g^{-1} and negligible loss in specific capacitance of 0.01025 F/g after each charge-discharge cycle (up to 8,000 cycles) in 3M KOH electrolyte. The asymmetric supercapacitor (ASC) device is fabricated by activated carbon (AC) as negative and Mo-doped ZnO as positive electrode material. Fabricated ASC device (Mo-doped ZnO@NF//AC@NF) shows a specific capacitance of 123 F g^{-1} at 1 A g^{-1} with capacitance retention of 75.6% after 8000 GCD cycles. A maximum specific energy of 39.06 Wh kg^{-1} at specific power of 7425 W kg^{-1} is observed. The astounding electrochemical performance of the 3D hierarchical nanostructure of Mo-doped ZnO electrode material indicates a promising candidate for efficient energy storage applications.

Keywords: Mo-doped ZnO; asymmetric supercapacitor; electrochemical performance; specific energy; specific power.

HYDROTHERMALLY SYNTHESIZED OF MULTI-DIMENSIONAL TiO_2 NANOSTRUCTURES BASED PHOTOCATALYST FOR CO_2 CONVERSION

Mohd Hasmizam Razali,[1] Uwaisulqarni M. Osman[1], Mohd Zul Helmi Rozaini[2], Mahani Yusoff[3]

[1]*Advanced Nanomaterials Research Group, Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, MALAYSIA*
[2]*Institute of Marine and Biotechnology, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, MALAYSIA*
[3]*Faculty of Bioengineering and Technology, Universiti Malaysia Kelantan Kampus Jeli, Karung Berkunci No.100, 17600 Jeli, Kelantan, MALAYSIA*
E-mail: mdhasmizam@umt.edu.my

Hydrothermally synthesized 0D, 1D and 2D titanium dioxide (TiO_2) nanostructures based photocatalyst was successfully synthesized using simple hydrothermal method. The sample was characterized using various techniques in order to study their physicochemical properties. The photocatalytic activity of synthesized nanostructures was investigated for CO_2 (carbon dioxide) conversion. Raman spectrum and x-ray diffraction (XRD) pattern show that the phase structure of synthesized TiO_2 nanostructures are anatase. Hollow spherical shape and elongated TiO_2 nanostructures was observed using transmission electron microscope (TEM) and the diameter of nanostructures was found to be 20-30 nm and 10 nm, respectively. Different dimensional of TiO_2 nanostructures possessed high surface area and pore volume. X-ray photoelectron spectroscopy (XPS) analysis revealed the formation of Ti^{4+} and Ti^{3+} species in the nanostructures TiO2 based photocatalyst in which could prevent the recombination of photo-generated electron, thus increased the electron transportation and photocatalytic activity of TiO_2 nanostructures for CO_2 conversion.

Iridium-Catalyzed C–H Borylation of CF_3-Substituted Pyridines

Ghayoor Abbas Chotana,[1*] Hafiza Tayyaba Shahzadi,[1] Saman Fatima,[1] Naseem Akhter,[1,2] Meshari Alazmi,[3] Alshammari Nawaf,[4] Kamaleldin B. Said,[5] Amer AlGhadhban,[6] Abdel Moneim E. Sulieman,[4] Rahman Shah Zaib Saleem,[1]

[1]Department of Chemistry and Chemical Engineering, Syed Babar Ali School of Science and Engineering, Lahore University of Management Sciences, Lahore-54792, Pakistan

[2]Department of Chemistry, Government Sadiq College Women University Bahawalpur-63100, Pakistan

[3]College of Computer Science and Engineering, University of Ha’il, P.O. Box 2440, Ha’il, 81451, Saudi Arabia

[4]College of Science, University of Ha'il, PO Box 2440, Ha'il - 81451, Saudi Arabia

[5]College of Medicine, University of Ha'il, Ha'il, Saudi Arabia

[6]College of Engineering, University of Ha’il, Ha’il, Saudi Arabia

Email: ghayoor.abbas@lums.edu.pk

Iridium-catalyzed C–H borylation of CF_3-substituted pyridines will be presented. The boronic ester group can be installed on the α, β, or γ position of pyridine by an appropriate substitution pattern. Sterically governed regioselectivity provides convenient access to a variety of CF_3-substituted pyridylboronic esters. These catalytic C–H borylation reactions were carried out neatly without the use of any solvent. Several functional groups, such as halo, ester, alkoxy, amino, etc., are compatible with this methodology. These pyridylboronic esters are amenable to column chromatography and the products were isolated in good to excellent yields. α-Borylated pyridines, although isolated in good yields, do not have a long shelf life. The boronic ester derivatives of these CF_3-substituted pyridines can serve as useful precursors in the synthesis regime.

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Ladder Type Bridged Thiazole Based Conjugated Electron Acceptors

Mohammed Al-Hashimi
Department of Chemistry, Texas A&M University at Qatar
P.O.Box 23874, Doha, Qatar

The field of π-conjugated organic semiconductors has significantly advanced over the past decade due to the extensive research that has been carried out for the fabrication of cost-effective, large-area, and flexible printed plastic electronics. Amongst the conjugated polymers, alternating donor-acceptor (D-A) units are widely utilized in the fabrication of organic photovoltaics (OPVs), and organic field-effect transistors (OFETs).
With specific modifications of the D-A moieties, one can progressively tune the energy levels and absorption properties as well as enhance the polymer backbone coplanarity and inter-chain connectivity, leading to the development of superior organic semiconductors, including higher carrier mobilities and photovoltaic power conversion efficiencies (PCEs).

Several conjugated copolymers based on the indacenodithiophene (**IDT**) donor unit have afforded impressive high mobilities and PECs as high as 8.27%, due to the enhanced inter-chain interactions facilitating the coplanarity of the polymer backbone. Most of the reported examples utilize the ladder type **IDT** core that is flanked with the electron-rich thiophene units. However, it has also been demonstrated that replacing the thiophene unit with other heterocycles such as selenophene effectively stabilizes the polymer lowest unoccupied molecular orbitals (LUMO), or introducing an electron-deficient thiazole moiety increases the electron affinity, and thus the large dipole on the heterocycle enhances both inter-chain π−π interactions and intra-chain π-conjugation. To the best of our knowledge, so far only two examples have been reported where the flanked thiophenes of the **IDT**-ladder have been modified.

Among the copolymers reported, the effect of substituting the thiophene unit with a thiazole moiety in the **IDT**-ladder to afford **IDTz** has been under investigated. In addition, di-2-thienyl-2,1,3-benzothiadiazole (**DTBT**) and 4,7-di(thien-2-yl)-5,6-difluoro-2,1,3-benzothiadiazole (**DTBTff**) have attracted considerable attention. It has been shown that the **DTBT** and **DTBTff** units can relieve the steric hindrance between the donor unit and the acceptor moiety, thereby stabilizing the highest occupied molecular orbital (HOMO) and LUMO energy levels, leading to excellent photovoltaic properties and, thus as a result, increasing the charge transport metrics and improving the PCEs.

To investigate the structure-property relationships underlying the charge transport of materials, there is still a need to develop new **IDTz**-based copolymers with different D/A combinations. Herein, we further develop the general design guidelines by synthesizing four new structurally related electron-accepting copolymers based on **IDTz-DTBT** and **IDTz-DTBTff** with the same backbone but different side chains and used for as new non-fullerene electron acceptors.

Luminescence and molecular modelling as tools to probe structure-property-performance relationships at molecular heterojunctions

Jenny Nelson, Mohammed Azzouzi, Flurin Eisner, Elham Rezasoltani and Jun Yan
Dept. of Physics, Imperial College London, UK,
Email: jenny.nelson@imperial.ac.uk

In a molecular photovoltaic device, charge separation and energy conversion result from the evolution of a photogenerated exciton into a charge separated state, in competition with recombination to ground. Recently, new molecular materials have led to steady increases in power conversion efficiency that now appoach 20%. To make further advances, we need to understand and isolate the effects of chemical structure, molecular packing, energetics and disorder on the competition between charge separation and recombination and hence on device efficiency. Electro- and photo-luminescence have proved to be valuable tools to probe the energy and dynamics of excited states involved in photoinduced charge separation, and to study structural and energetic disorder at molecular interfaces. The combination luminescence with other spectroscopic techniques, transient electrical measurements and computational modelling can be effective in helping us to understand how chemical and physical structure control the basic mechanisms of a photovoltaic device. Such an approach can be used to study the properties and role of charge transfer states, and the impact of structural and energetic disorder. We show how an integrated computational model allows different experimental measurements to be reconciled within a single picture and helps to show how the properties of interfacial statescontrol the device [1]. We use our results to consider the ultimate limitations placed on solar to electric conversion by the molecular nature of the materials.

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MAKING PRINTABLE, MECHANICALLLY AGILE ELECTRONICS AND OPTO-ELECTRONCS A REALITY. POLYMERS, HETEROJUNCTIONS, AMORPHOUS OXIDES, AND SOLAR CELLS.

Tobin J. Marks[1]
[1]Department of Chemistry, the Center for Hierarchical Materials Design, the Materials Research Center, and the Institute for Sustainability and Energy, Northwestern University, Evanston, IL 60208-3113 USA
E-mail: t-marks@northwestern.edu

This lecture focuses on the challenging of designing, realizing, characterizing, hybridizing, and understanding new, dissimilar materials families for unconventional electronics and opto-electronic devices to provide a number of targeted applications. Fabrication methodologies to achieve these goals will ultimately include high-throughput, large-area, high-resolution, environmentally benign printing and coating techniques. Materials design features to be discussed include: 1. Rationally designed high-mobility mechanically agile p- and n-type soft matter semiconductors for organic CMOS; 2. Polycrystalline and amorphous oxide semiconductors for printable, transparent, and mechanically agile electronics, 3. Hybrid organic + inorganic semiconductors for high carrier mobility, optical transparency, and mechanical agility, 4. Combining these materials sets to rapidly fabricate scalable, high-performance thin-film complementary transistor and photovoltaic devices for switching, sensing, energy storage, and energy conversion.

MARINE BIOMATERIALS DERIVED FROM FRINGESCALE SARDINIELLA BONES AS ADVANCED SUNSCREEN MATERIALS

Mohd Zul Helmi Rozaini[1,3*], Md Uwaisulqarni Osman[2] and Mohd Hasmizam Razali[2]

[1]*Institute of Marine and Biotechnology, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, MALAYSIA*

[2]*Faculty of Science and Marine Environment, 21030 Kuala Nerus, Terengganu, MALAYSIA*

[3]*Faculty of Fisheries and Food Sciences, Universiti Malaysia Terengganu, 21030, Kuala Nerus, MALAYSIA*

Email: zulhelmi@umt.edu.my

A novel biological or synthetic substance derived from marine waste by-product or biomaterials have been identified can produce good sunscreen materials. Fish processing industry has led to large amounts of waste every year around the world. However, waste from the fish bone contains valuable compound such as hydroxyapatite (HAp). Fish bones are natural resources and have an attractive added value which contains HAp that can potentially be used as hybrid sunscreen. Therefore, Fringescale sardinella (Valenciennes, 1847) bones have been discovered and HAp was synthesized to be applied in cosmeceuticals applications. The properties of HAp from Fringescale sardinella bones have been characterized with Fourier Transform Infrared Ray (FTIR) and Cytotoxicity test. The emulsions have been formulated and tested under Ultraviolet Visible (UV-Vis) Spectroscopy. Results had indicated that fish bones doped with $FeCl_2$ shows higher tendency as sunscreen compared to $MnCl_2$ and unmodified bones. Thus, the utilization of waste from fish bones will not only adding value to the by-products, but also help in reducing pollution to the environment and preventing from global warming. Hence, formulation on emulsion synthesized from fish bone is designed as a new hybrid innovation in cosmeceutical products and boost up the efficiency of skin prevention from UV radiation.

Keywords: Marine based, biomaterials, sunscreen, fishbones, frigescale sardiniella

NANOPARTICLES, METAL-ORGANIC FRAMEWORK, & MICROFLUDICS-NOVEL ANALYTICAL APPLICATIONS

Haider A. J. Al Lawati[1]

Department of Chemistry, College of Science, Sultan Qaboos University, Oman

Microfluidic is a technique in which channels of sub-millimetre dimensions are etched on a solid substrate to perform various analytical steps such as sample preparation, mixing, reaction, analytical separation, detection, signal evaluation and quantification. The use of a miniaturized platform consumes minute amounts of chemicals and reduces the cost of analysis. Additionally, microfluidic methods reduce analysis time and increase sample throughput.

Nanomaterials have received great attention due to their high surface area and energy along with the quantum size effect, they are characterized by their unusual mechanical and optical properties, special catalytic activity and high adsorption capacity.

Metal organic frames (MOFs) are special porous inorganic polymers containing cationic central parts, which connected by certain multi-dentate organic bridges. These materials have several advantages such as; Large surface area, uniform and large pore sizes, great stability, and a flexible structure with high versatility in chemical composition.

In this presentation we will discuss the utilization of Nanomaterials and MOF in microfluidics as media for enhancing the sensitivity of analytical systems and improving the stability of some enzymes. We will discuss also the utilization of MOF as media for separation and for extraction inside microfluidic chips.

New Highly Efficient TiO_2-based photocatalysts for Phenol degradation.

Aboubakr M. Abdullah
Center for Advanced Materials
Qatar University, Doha 2713, Qatar

Abstract: Different BN/TiO_2 nanocomposites were prepared hydrothermally, and their ratio was optimized to get the best photocatalytic performance towards phenol degradation. They were characterized by x-ray photoelectron spectroscopy, x-ray diffraction, Fourier transform infrared spectroscopy, thermal gravimetric analysis, scanning and transmission electron microscopies coupled with energy dispersive x-ray units, BET surface area, and UV-Vis diffuse reflectance. The bandgap energy was reduced from 3.35 to 2.95 eV due to the formation of the B−O−Ti bond. This allowed the exploitation of the visible light and inhibited the TiO_2 e^-/h^+ recombination, and consequently, the photocatalytic activity of TiO_2 was dramatically improved. Almost 90 % mineralization of 20 ppm phenol solution was achieved within 30 min under simulated sunlight. The as-prepared composite showed excellent stability and reusability. Mechanistic analysis indicated that $O_2^{\cdot -}$ and h^+ played a crucial role in phenol degradation. The nanocomposite′s biocompatibility and environmental impact were evaluated by analyzing its potential toxicity in vivo using the zebrafish embryos. 96-hpf acute toxicity assays, including the mortality rate assay (to obtain the LC50 values) and teratogenic assays (to obtain the No Observed Effect Concentration, NOEC) was conducted. The LC50 value for BN/TiO_2 was 482.5 mg L^{-1}, and the NOEC was 100 mg L^{-1}. Based on LC50 value and according to the Fish and Wildlife Service (FWS) acute toxicity rating scale, the photocatalyst is “practically not toxic.”

NOVEL NAPHTALENE DIIMIDE BASED INTERLAYER MATERIALS FOR ORGANIC AND PEROVSKITE PHOTOVOLTAICS

Bob C. Schroeder[1]

[1] Department of Chemistry, University College London, London WC1H 0AJ, UK
Email: b.c.schroeder@ucl.ac.uk

Organic and hybrid organic-inorganic photovoltaic devices have come a long way, both with regards to power conversion efficiencies and device stability, a development largely made possible by the synthesis of new higher performing organic semiconductors and more elaborate device architectures. A major component responsible for the dramatically improved efficiencies are interlayer materials that improve charge extraction from photovoltaic devices. While numerous p-type interlayer materials are commercially available, most notably PEDOT:PSS, cathodic interlayer materials are still scarce. The limited availability of n-type organic semiconductors is two-fold. On the one hand the chemistry often encountered with electron deficient materials is challenging, making the synthesis of new structures difficult. On the other hand the notorious reactivity of n-type organic semiconductors towards oxygen makes their handling and long-term storage more demanding than for their p-type counterparts.

Herein we will discuss the synthesis of a series of naphthalene diimide based conjugated polymers their application as cathode interface layer materials in organic and perovskite photovoltaics, yielding power conversion efficiencies (PCE) in excess of 16%.[1] We will show how the synthetic design and processing of these novel interlayer materials can be exploited to reduce trap-assisted carrier recombination and increase the built-in potential, simultaneously enhancing photovoltaic parameters. We will then take the structural design a step further and outline a synthetic approach towards water-processable and air-stable self-dopant organic n-type conductors, which we believe will form the backbone of the next generation interlayer materials in plastic electronics.

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POLYMER CAPSULE SHELLS WITH DYNAMIC COVALENT BONDS: DESTRUCTION AND FUSION ON DEMAND

Yifei Wang,[1] Emily Pentzer[1,2]

[1]Department of Materials Science and Engineering, [2]Department of Chemistry
Texas A&M University, College Station, TX 77843

Encapsulation of liquids is important across many applications, including foodstuffs, cosmetics, payload delivery, and so on, and can also be used as an attractive route for overcoming cumbersome handling of viscous liquids or accommodating volume change upon solid-liquid phase changes. The three common routes to prepare capsules with liquid cores are the soft template method (e.g., interfacial polymerization in an emulsion), the hard template method (e.g., impregnation of solid hollow shells with liquid), and the use of microfluidics. Of these, the soft template method is perhaps the most scalable and is amenable to tuning of core and shell materials.

The Pentzer group has developed alkylated graphene oxide (GO) nanosheets as Pickering surfactants for the stabilization of non-aqueous emulsions (e.g., oil-in-oil, ionic liquid-in-oil), and demonstrated the preparation of capsules by interfacial polymerization between a diamine and a diisocyanate [1-3]. When the core of these capsules is an ionic liquid, they have application in energy storage, solvent remediation, and uptake of gaseous carbon dioxide. This presentation will focus on the integration of dynamic covalent bonds, specifically hindered urea bonds, into the shell of the capsules. [4]. Upon preparation, reaction between monomers with secondary amines and isocyanates produce individual capsules that are stable to isolation; however, upon heating of the capsules the hindered urea bonds undergo the reverse reaction, yielding diamines and isocyanates. If the capsules are heated in the presence of primary amine, the capsule shells are destroyed. Alternatively, if the capsules are collected and heated, bond exchange between capsule shells produces a monolith. The temperature required for activating these transformations is dependent on the identity of the secondary amine as well as that of the liquid core, and the proposed mechanism for morphology change is supported by variable temperature FTIR measurements.

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POLYMER STABILIZED METALLIC NANOPARTICLES: AN EFFICIENT AND SELECTIVE PLATFORM FOR SENSING DRUGS AND PESTICIDES

Muhammad Imran Malik
Third World Center for Science and Technology, H.E.J. Research Institute of Chemistry,
International Center for Chemical and Biological Sciences (ICCBS), University of Karachi,
Karachi 75270, Pakistan
E-mail:*mimran.malik@iccs.edu; m.imran.malik1gmail.com

The development of novel sensors using metal nanoparticles (MNPs) for detection of organic/bio compounds is a subject of recent interest of many scientists. Numerous nanocomposites having varying molecular recognition and signal transduction properties have been synthesized for rapid and accurate determination of chemical contaminants in different matrices such as water, food, and biological fluids etc. In this context, several synthetic polymers such as polypropylene glycol, poly (2-vinyl pyridine), poly(ethylene oxide-b-caprolactone), poly(styrene-b-2-vinylpyridine), poly(2-vinlypyridine-b-methyl methacrylate) etc. have been used by our group for stabilization of MNPs which were subsequently applied for the recognition of number of analytes such as metals, pesticides, drugs, etc.[1-7] These polymers not only stabilize MNPs but also make them selective and sensitive towards a particular analyte owing to presence of different functional groups on them. Polymers with lone pair donating groups are the potential candidates for the stabilization of MNPs due to their ability of chelation. A common feature of all these polymers is presence of nitrogen, oxygen, or sulfur atoms in their repeat unit that can donate electron pair for chelation of the metals. In this lecture, we will discuss the selectivity of different functional groups on the polymers for stabilization of the MNPs and subsequently their recognition peculiarity for different drugs and pesticides. The caveats and merits of different sensors in context of their limit of detection, stability, recognition potential in presence of other interferents (drugs, slats, metals, and pesticides), and in real samples (biological, ecological, and environmental) will be demonstrated.

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QUINOLONE ANTIBIOTIC LOADED MESOPOROUS SILICA NANOPARTICLES AS EFFECTIVE ANTIMICROBIAL AGENT AGAINST RESISTANT PATHOGENS

Urooj Haroon[1], Muhammad Hashim Zuberi[2]

[1] *Chemistry Department, Federal Urdu University for Arts Science and Technology, Karachi, 74000, Pakistan*
[2] *Environmental Sciences Department, Sindh Madressatul Islam University, Karachi, 74000, Pakistan*
uroojharoon@fuuast.edu.pk

PEG coated mesoporous silica nanoparticles were prepared and characterized for the purpose of antibacterial applications. The particles were synthesized by the hydrolysis of tetraethyl orthosilicate (TEOS) in methanolic medium under catalysis by tri ethyl amine using surfactant CTAB as a structure directing agent. Two quinolone antibiotics; levofloxacin and sparfloxacin were loaded in the pores of the surface modified SiNPs. Structural studies were carried out using UV, FT-IR spectroscopy, Dynamic light scattering, Scanning Electron Microscopy and X-Ray Diffraction techniques. PEG-levo and PEG-spar particles appeared as rectangular shaped nano-objects between 241-300 nm and 241-283 nm in size respectively. The amount of drug loaded was found to be 97-98 %. Comparison of antimicrobial profile of levofloxacin and sparfloxacin before and after loading was performed against six different bacterial clinical isolates including *Staphylococcus epidermidis, Bacilus subtilus, Escherichia coli, Psuedomonas aeuroginosa, Staphylococcus aureus* and *Klebsiella pneumoniea*. Results showed that PEG-spar exhibited slightly increased activity against *P. aeuroginosa* while activity was very high against *S. aureus* as compared to Sparfloxacin. Similarly PEG-levo showed prominent activity against *S. aureus* only as compared to the parent drug. Particles exhibiting specific activity against targeted pathogens can be utilized as pathogen specific antibiotics for targeted treatment of bacterial infection caused by resistant pathogens. One of the major advantages of lower spectrum antimicrobial agent is that they would not disturb the human microbiome and resistance would be slower to develop.

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Rational Design of Catalytic Materials for Clean Energy Generation and Storage Applications

Ahsanulhaq Qurashi *

Department of Chemistry, Khalifa University of Science and Technology, Main Campus, Abu Dhabi, P.O. Box 127788, United Arab Emirates

To advance the progress of clean energy, various promising new materials-based devices and systems have been systematically investigated in past few years. In this talk, we will discuss various potential electrode materials for hydrogen and oxygen production through water splitting, CO_2 conversion process and other clean energy production and storage applications. Also, discuss recent progress on integrated systems to photo-electrolysis, artificial photosynthesis such as CO_2 conversion into value-added chemical reduction-products, where advancements in new catalysts and solution-processed inexpensive PV devices can certainly enrich the overall performance of the renewable production of solar fuels, including solar driven carbonaceous fuels. Finally, an overview of challenges, frontiers and opportunities of materials for energy conversion and storage systems will be conversed.

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SMART COVALENT ORGANIC FRAMEWORKS

Ali Trabolsi[1]

[1]*New York University Abu Dhabi*

Smart materials that can reversibly change their properties in response to an external stimulus such as light, pH, heat, redox reagents, and/or small molecules are currently the thriving topic of research due to their wide range of applications. Porous framework materials such as covalent organic frameworks (COFs) are well known for their applications in various challenging fields. By adding a property that responds to stimuli, they become even more powerful and can change their properties as needed. Since they are built from organic building blocks, we decided to functionalize them with the desired reactive components to bring out the responsive behavior. Careful selection of functionalization techniques maintained the active surfaces and porosity, while precise functionalization enabled responsiveness to stimuli. We have successively presented the development of such stimuli responsive smart covalent organic frameworks bearing physical and chemical stimulus-responsive components and demonstrated their immense application potential. The attachment of families of responsive components such as azobenzene, viologen, and spiropyran groups has laid the foundation and incorporated the photosensitivity of the scaffold including chromic behavior, which has then been further exploited for the delivery of various molecular cargoes. The incorporation of magnetic properties through the incorporation of magnetic nanoparticles is another unique feature in the development of magnetically responsive framework composites. Our most recent example demonstrates the successful development of a glucose-responsive covalent organic framework for the selective delivery of insulin, a major breakthrough in the future treatment of diabetes.

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SOLVENT-FREE ORGANIC LIQUIDS: OPPORTUNITIES OF A NEW ORGANIC SOFT MATERIAL

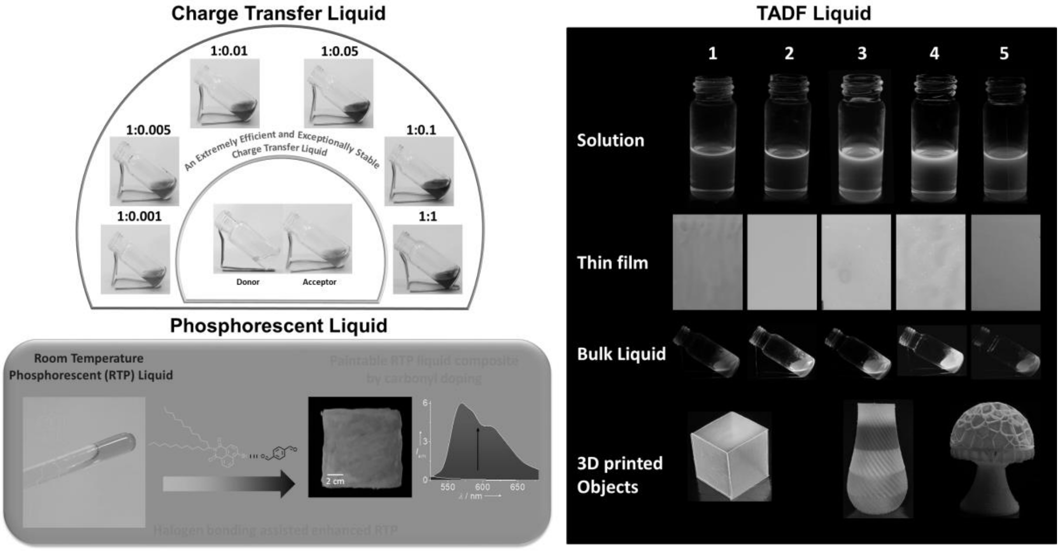
Santhosh Babu Sukumaran[1]

1Organic Chemistry Division, National Chemical Laboratory (CSIR-NCL),

Dr. Homi Bhabha Road, Pune-411008, India

Email: sb.sukumaran@ncl.res.in

Solvent-free organic liquids have been developing as a new soft material parallel to solute-solvent-based systems, where the solvents control the solute molecules exclusively.[1] In molecular systems studying charge transfer, energy/electron transfer, etc., solvent molecules and thereby polarity of the medium creates a drastic difference in the efficiency. Hence to study the ground and excited-state properties of functional chromophores, our research group extended our research to develop many solvent-free organic liquids that exhibit unprecedented photophysical properties compared to the solid/crystalline analogs. The ground-state donor-acceptor interactions have been modulated to develop a highly stable and efficient charge-transfer liquid with very low loading of the acceptor; 1 acceptor molecule for 1000 donor molecules.[2] Another study explored the room temperature phosphorescence features of a solvent-free organic liquid phosphor in air.[3] In a recent development, thermally activated delayed fluorescence of a solvent-free organic liquid exhibiting monomer-like optical features in bulk was investigated.[4] Organic TADF liquids have been used for developing tunable emission hybrid liquids through energy transfer and found helpful in 3D printing applications.



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SUPRAMOLECULAR STRUCTURES WITH INTRINSIC MICROPOROSITY FOR “ON-DEMAND” SEPARATIONS: ONE STEP CLOSER TO INDUSTRIAL TRANSLATION

Niveen M. Khashab[1]
[1]Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Saudi Arabia
niveen.khashab@kaust.edu.sa

Nature embraces the principles of supramolecular chemistry, exploiting noncovalent interactions and coordination chemistry in various ways to facilitate all biological processes. Inspired by nature, the assembly of complex synthetic systems in both solution and the solid state is becoming increasingly feasible. This often requires that known systems be modeled, explored, and fine-tuned in order to develop further systems of even higher complexity. Examples include the construction of globular self-assembled molecular capsules, which have potential applications as drug delivery agents, gas storage containers and catalytic nano-reactors. Moreover, fine-tuning porosity in such assemblies have expanded the scope of these systems to include gas and petrochemicals separation. Our approach to this class of functional self-assembled structures includes employing a "window construction" technique, which provides a new class of materials with intrinsic microporosity. Simple hydrogen bonding and/ or metal coordination were employed to construct a library of these suprastructures, which showed excellent selectivity towards guest separation together with easily tunable pore size. This talk will present an overview of the systems obtained so far and their applications in energy intensive separations as well as our future plans for industrial translation.

SYNTHESIS, SPECTROSCOPY AND CONDUCTIVITY STUDIES OF 4-NITROPHENYL THIOSEMICARBAZIDE MIXED WITH CARBOXYMETHYL CELLULOSE POLYMER

Uwaisulqarni M. Osman[1,2], Zuliana S. Zulkifli[1], Khadijah H. Kamarudin[1,2], Mohd Hasmizam Razali[1,2], Mohd Zul Helmi Roziani[3]

[1]Faculty of Science and Marine Environment, Universiti Malaysia Terengganu,
21030 Kuala Nerus, Terengganu, Malaysia
[2]Advanced Nano Materials Research Group (ANOMA), Ionic State Analysis (ISA) Laboratory,
Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia
[3]Faculty of Fisheries and Food Science, Universiti Malaysia Terengganu,
21030 Kuala Nerus, Terengganu, Malaysia
E-mail: uwais@umt.edu.my

A compound, 4-nitrophenyl thiosemicarbazide was prepared from 4-nitrophenyl isothiocyanate and hydrazine hydrate in ethanol. The compound was characterized by CHNS elemental analysis, Fourier Transform Infrared spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy and Nuclear Magnetic Resonance (NMR) spectroscopy. The FTIR spectra show that the compound exhibit the thione-thiol tautomerism. Two peaks were appeared in electronic spectra due to both $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions. The theoretical band gap was measured using Density Function Theory (DFT) level with a 6-311G (d,p) basic set. Finally, a solution casting technique was used to make polymer electrolytes films composed of carboxymethyl cellulose (CMC) polymer, propylene carbonate as a plasticizer and 4-nitrophenyl thiosemicarbazide compound as a dopant to measure their conductivity using Electrochemical Impedance Spectroscopy (EIS). The conductivity was observed for 4-nitrophenyl thiosemicarbazide at 3.1826×10^{11} $\mathrm{Scm^{-1}}$.

THE ELECTROCHEMICAL REDUCTION OF CO_2 TO VALUABLE CARBON IN ALKALI CARBONATE MELTS

Mohammad Danish,[1] **Omnya Abdalla,**[1] **Ammar Elhoweris,**[1] **Roneta Chaliulina,**[1] **Amer Hakki,**[1] **Jonathan Mwanda**[1,2]

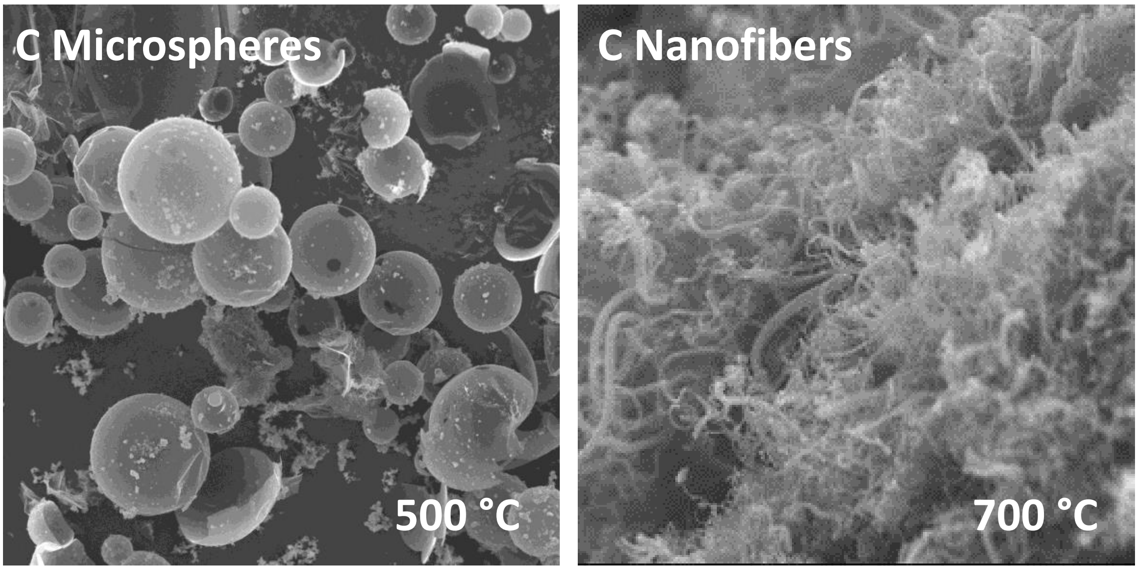
[1]*Gulf Organisation for Research and Development, Qatar Science and Technology Park, Doha, Qatar*

[2]*Corresondence and requests should be addressed to J.M. (e-mail: j.mwanda@gord.qa)*

Carbon dioxide is one of the most abundant greenhouse gases that contribute significantly to current and projected adverse global climate change. Various strategies to mitigate increased CO_2 concentrations in the atmosphere include carbon capture and utilization technologies that enable the capture of CO_2 and convert it to valuable carbonaceous materials. In this study, electrochemical reduction of CO_2 to carbon employing a eutectic mixture of Li-Na-K molten carbonates is presented and investigations into the influence of synthesis conditions and electrochemical parameters on the resultant carbon morphology is also explored. Variation of the electrochemical synthesis parameters such as current density, voltage, molten salt temperature, synthesis steps and the electrode material, were studied to elucidate the resultant carbon structures (graphene, carbon nanofibers, and spheres).

The distinctive characteristics of the electrolytic system was analyzed using cyclic voltammetry to determine the essential redox (oxidation-reduction) reactions to ensure optimum conditions for carbon synthesis. An array of characterization techniques were also used to examine the synthesized carbons such as SEM, EDS, FT-IR, and XRD.

At lower temperatures i.e., 500ºC, the dominant structure was spherical carbon with some amorphous carbon, while at higher temperature of 700ºC, the major structures were carbon nanofibers and nanotubes. The produced spherical carbon showed adequate contaminant adsorption capabilities demonstrated by a high percentage of methylene blue removal from water. While the produced carbon nanofibers have multiple applications including superior properties as an energy storage material for both lithium and sodium ion batteries.



The Role of Graphene on the Thermal Stability and Plasmonic Formation in Aluminium Nanocomposites

Khaled Youssef
Materials Science and Technology Graduate Program, Qatar University, Doha, 2713, Qatar

Abstract

One route to facing energy-related challenges and enhancing environmental sustainability is through fundamental material science and engineering approaches. Improving energy efficiency, reducing harmful emissions, and furthering environmental sustainability can be attained by synthesizing and fabricating novel lightweight materials with enhanced properties. Nanocrystalline (nc) metals have strengths exceeding those of coarse-grained and even alloyed metals and are expected to be utilized in many energy and structural related applications. However, nanocrystalline materials are prone to grain growth at lower temperatures than their conventional counterparts. We synthesized thermally stable, lightweight, aluminum-lithium-graphene nanocomposites with superior mechanical properties. The synthesis process was also developed to produce these novel materials in the form of nanoplatelets that exhibited plasmonic characteristics with anisotropic morphologies using a simple ball-milling technique. Structural analysis using SEM and TEM revealed that the nanoplatelets are single-crystals with a hexagonal platelet-like morphology of a ~300-500 nm diagonal and a ~60 nm thickness. Furthermore, the UV-Vis spectroscopy of the hexagonal Al-based nanoplatelets exhibited plasmonic resonance absorption bands in the UV region at a wavelength of 214 nm and 345 nm. This presentation illustrates the feasibility of building epitaxial plasmonic metal-graphene systems inside bulk metal-graphene composites using a simple milling process.

Short Biographical Sketch: Dr. Khaled Youssef

Materials Science and Technology Graduate Program, Qatar University, P.O.Box 2713. Doha, Qatar
E-mail: kyoussef@qu.edu.qa
Website: http://qufaculty.qu.edu.qa/kyoussef
ORCID: https://orcid.org/0000-0001-9850-5223

Dr. Khaled Youssef is an Associate Professor and the Coordinator of the Materials Science and Technology Graduate Program, Qatar University. Dr. Youssef obtained his Ph.D. in Materials Science and Engineering from North Carolina State University, USA. His research focuses on the synthesis, characterization, and properties of nanocrystalline materials, high-entropy alloys, and nanostrcturing/nanocompositing effects in thermoelectric materials. For many years, Dr. Youssef was the co-director of the NSF/IUCRC Silicon Solar Consortium at North Carolina State University. He has developed in-situ consolidation during milling techniques to produce artifact-free bulk nanocrystalline materials with superior properties. Dr. Youssef is granted several NPRP (Qatar), NSF (USA), and DOE (USA) awards. In addition, he has published over 70 peer-reviewed articles that received more than 4000 citations. Dr. Youssef also advised many Ph.D. and MSc students, and he is an editorial board member of many journals.

TRIS(5,7-DIPHENYL-8-QUINOLINOLATO) INDIUM(III) COMPLEX: SYNTHESIS AND CHARACTERIZATION

Usama A. Al-Zaabi, Saleh N. Al-Busafi, FakhrEldin O. Suliman

Department of chemistry, Sultan Qaboos University, Muscat, Sultanate of Oman

E-mail: s5399@student.squ.edu.om

8-quinolinolate metal-chelate complexes are one of the most powerful optoelectronic materials for the organic light-emitting diodes (OLEDs). Because of their importance, research efforts have been concentrated on studying this class of materials as bulk materials since 1987[1] as well as the nanomaterials in recent years. Despite the large number of studies devoted to the aluminum complex (Alq_3) from various visual angles, few studies have been performed so far to systematically investigate the indium counterpart and its derivatives. Therefore, this contribution focuses on the molecular structure, photophysical and thermal properties of tris(5,7-diphenyl-8-quinolinolato) indium(III) complex, $In(5,7\text{-}Phq)_3$.

The 8-HQ derivative (5,7-diphenyl-8-hydroxyquinoline) was successfully synthesized *via* Suzuki cross-coupling reaction before the synthesis of $In(5,7\text{-}Phq)_3$ complex and their molecular structures were confirmed using single-crystal X-ray crystallography. The $In(5,7\text{-}Phq)_3$ complex was characterized using various spectroscopic techniques, including Fourier-Transform Infrared (FT-IR) spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy, photoluminescence (PL) spectroscopy, and thermogravimetric analysis (TGA).

The single-crystal X-ray structure of the complex indicates that the three 5,7-diphenyl-8-hydroxyquinoline ligands are arranged in a *meridional* configuration about the central metal In^{3+} ion, and the complex is distorted from ideal octahedral geometry. The unit cell parameters obtained are a = 14.670(3) Å, b = 23.450(5) Å, c = 15.970(3) Å, a = 90°, β = 112.30(3)° and γ = 90° which indicates the structure is monoclinic, $P2_1/c$, with Z = 4. The FT-IR spectroscopic analysis confirms the formation of the organometallic $In(5,7\text{-}Phq)_3$ complex through the existence of the stretching vibration of the In–O and In–N bonds in the spectrum. The FT-IR peak at 429 cm^{-1} is assigned to the In–N stretching vibration, while the peaks at 662, 552, and 513 cm^{-1} arise from the stretching vibrations of the In–O bonding. A broad absorption band at 406 nm was observed in the UV-vis spectrum of the complex which is assignable to π-π^* transitions. The PL of the complex showed a red shift in emission wavelength to 535 nm in chloroform at room temperature (298 K). Furthermore, the complex thin film and powder samples showed emission wavelengths at 545 and 552 nm, respectively. The bandgap energy (E_g) determined from the Tauc plot method is 2.35 eV smaller than that reported for the Alq_3 and Gaq_3[2]. The results of the fluorescence decay of the $In(5,7\text{-}Phq)_3$ complex in chloroform at 298 K show that the decay fits the biexponential model with two lifetimes of $\tau_1 =$ 32.87 ns (longer) and $\tau_2 =$ 5.99 ns (shorter). The TGA results show that the complex degraded at three stages at 331, 485, and 603 °C and decompose at 650°C.

In this study, $In(5,7\text{-}Phq)_3$ complex was synthesized and characterized optically and thermally. Considering its interesting photophysical properties, the complex is a potential light-emitting material that may find applications in optoelectronic devices.

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Tunable Functional 3D-Covalent Organic Framework Membranes for Water Remediation

Dinesh Shetty

Department of Chemistry & Center for Catalysis and Separations (CeCaS), Khalifa University, PO Box 129188, Abu Dhabi, UAE

Crystalline porous covalent materials such as covalent organic frameworks (COFs) have gained significant attention in the scientific community for a wide array of applications because of their attractive physical and chemical properties.[1,2] However, the functional tunability of COFs, which is highly important for many critical applications, is generally limited to the strategic selection of molecular building blocks.[3] In this regard, a simple and one-step facile method to tune the physiochemical properties of free-standing membranes is fundamentally attractive and highly useful for technology transfer. Recently, we have successfully synthesized the free-standing 3D-COF membranes and introduced a novel pre-synthetically controlled framework growth strategy to tune the hydrophobicity of the resulting membranes without changing the building blocks (Fig. 1).[4] Notably, the solvent change from chloroform to ethyl acetate switches the membrane property from hydrophilic (water contact angle 60°) to hydrophobic (water contact angle 142°) nature. The hydrophobic 3D-COF membrane selectively passes oil molecules from an oil-water emulsion with a gravitational flux of 1536 L m-2 h-1. Building on the findings, we have developed multiple COF-based membrane materials (both pristine and mixed-matrix membranes) and tested their efficiency in different water purification techniques, including nanofiltration, ultrafiltration, and reverse electrodialysis. We successfully removed toxic molecules, metals, and ions from the polluted or saltwater. Results obtained by these novel materials are significantly superior to those from most materials reported previously. The high efficiency and ease of implementation of our materials demonstrate the advantages of our findings and bode well for the development of COF-based membrane materials for various applications.

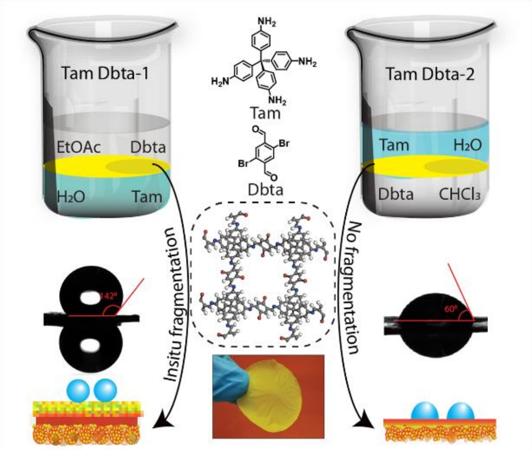

***Figure 1**. Demonstration of a novel pre-synthetically controlled framework growth strategy to tune the hydrophobicity of the 3D-COF membranes without changing the building blocks or post-synthetic modifications. The hydrophobic 3D-COF membrane was utilized for the demulsification of an oil-water mixture.*

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Water, Energy, and Food Sustainability

2D Nitride MXenes for Electrochemical Energy Storage and Conversion

Abdoulaye Djire

Assistant Professor, Department of Chemical Engineering, Department of Materials Science and Engineering (Affiliated), Texas A&M University, College Station, TX 77843

adjire@tamu.edu

Abstract

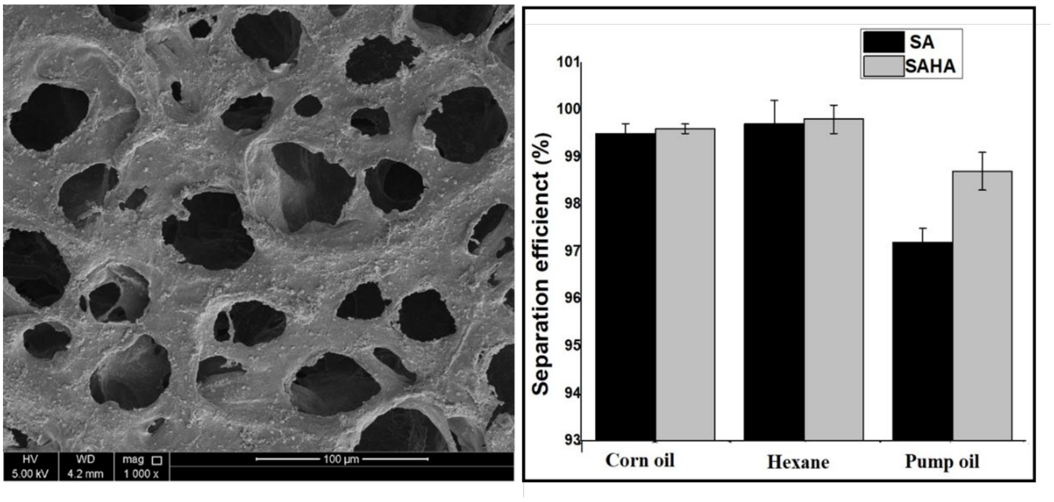
The large-scale shift towards renewable energy requires the ability to reliably store electrochemical energy. This technology is still limited in terms of performance, cost, and/or ease of utilization. Two-dimensional (2D) materials have been explored as low-cost, high-performing catalysts and electrodes for reliably storing electrochemical energy. Of these 2D materials, a special class of carbides and nitrides, known as MXenes, have gained popularity due to their high tunability, conductivity, and high surface area-to-volume ratio. From these MXenes, the carbide formation has been the most vastly studied, but the nitride MXene has been theorized to perform better due to their higher electronic conductivity. In this presentation, I will present on the oxygen-assisted molten salt fluoride etching synthesis method developed in my lab to produce phase-pure Ti_2N nitride MXene. Along with this, I will provide evidence of the enhanced capabilities of the nitride MXene against the benchmark carbide MXene, Ti_3C_2, when applied in the nitrogen reduction reaction (NRR), hydrogen evolution reaction (HER), carbon dioxide reduction reaction (CO_2RR), electromagnetic interference (EMI) shielding, and supercapacitor applications. In each of these fields, the enhanced performance is directly related to the capability of the Ti–N to attract electrons to the structure which consequently allows the material to engage more readily and rapidly with the electrolyte ions. I will wrap up by discussing the future directions in the field of MXenes that require further attention for the advancement of 2D materials in electrochemical energy storage and conversion systems.

BIOPOLYMER BASED NANOCOMPOSITE AEROGEL: PREPARATION, STRUCTURE AND APPLICATION IN WASTE WATER REMEDIATION

Sneha Bhagyaraj* **Anton Popelka, Peter Kasak, and Igor Krupa***
Center for Advanced Materials, Qatar University, P.O. Box 2713 Doha, Qatar
**Email: sneha.bhagyaraj@qu.edu.qa ; igor.krupa@qu.edu.qa*

Abstract

Designing environmental friendly materials and approaches for addressing various pollution-related issues, especially water pollution, is in high demand [1]. Here, we report an environmentally friendly, low-cost and stable sodium alginate (SA)-halloysite clay (HA) composite aerogel (SAHA) fabricated via a two-step synthesis procedure, including ionic crosslinking and freeze drying. Detailed morphological analysis of the SAHA aerogels revealed a three-dimensional porous microstructure with uniformly dispersed halloysite nanotubes (HA) within the alginate matrix. The elemental composition of the hydrogels investigated using energy dispersive X-ray spectrometry (EDX) revealed the presence of minerals, such as magnesium, sodium, aluminum and silicon, in the SAHA aerogels. The aerogel showed an amphiphilic character towards water and oil in air, while it exhibited underwater superoleophobicity. Through the incorporation of halloysite clay nanotubes, the SAHA aerogels showed improved separation efficiencies for corn oil, hexane and pump oil of 99.6%, 99.8% and 98.7%, respectively. The reusability of the SAHA aerogel was also better compared to neat aerogel (SA). The as prepared aerogel also showed excellent adsorption of boron from desalinated water with an efficiency of 90.4 %, and adsorption capacity of 510 mg/g in optimum pH=8 at room temperature. The excellent oil/water separation and multiple performances make the SAHA aerogel an interesting candidate for effective cleaning of oil spills and practical applications in water recycling.



Keywords: alginate aerogel; halloysite; nanocomposite; oil/water separation; boron removal

Acknowledgement: This work is supported by the Qatar University grant QUCG-CAM-22/23-582.

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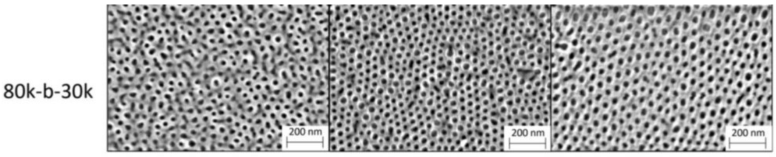
BLOCK COPOLYMER MEMBRANES WITH HIGHLY UNIFORM PORES FOR ADVANCED OIL/WATER SEPARATION IN OIL AND GAS INDUSTRY

Mohammad K. Hassan[1], Shifa M.R. Shaikh[1,2], Daniel Weller[3], Moustafa Zagho[3], Yara Elgawady[1], Khadar B. Shaik[4], Xiaodan Gu[3], Sergei Nazarenko[3], Mustafa Nasser[2], Samer Adham[5], Mariam Al-Maadeed[1,6], Alamgir Karim[4]

[1]Centre for Advanced Materials, Qatar University, Doha, Qatar
[2]Gas Processing Center, College of Engineering, Qatar University, Doha, Qatar
[3]School of Polymer Science and Engineering, University of Southern Mississippi, USA
[4]Department of Chemical and Biomolecular Engineering, University of Houston, USA
[5]ConocoPhillips Global Water Sustainability Centre, Qatar Science and Technology Park, Qatar
[6]Materials Science and Technology Program, Qatar University, P. O. Box 2713, Doha, Qatar
E-mail: mohamed.hassan@qu.edu.qa

Oil and gas industries worldwide are constantly developing advanced systems to enable the treatment and reuse of wastewater. Oil and grease represents the main component of wastewater, and their removal is considered a major challenge. Current treatment methods include physical, chemical, and electrical schemes, to remove dissolved pollutants and permit water reuse. However, conventional separation techniques pose major challenges in the treatment of produced water, as they are less efficient, energy-intensive, and have expensive upscaling requirements. Membrane separation techniques prove promising for efficient large-scale produced water treatment. Improvements in ultrafiltration and nanoporous membrane designs aim at facilitating high rejection rates, higher fluxes, reduced fouling tendencies and effective upscaling of the production process. Block copolymers comprise a novel class of polymers that can self-assemble into ordered, chemically distinct microdomains with sizes ranging from 3-50 nm.

This talk will highlight our efforts at Qatar University, which aim to fabricate porous block copolymer (BCP) membranes, as shown in the enclosed morphology pictures, using different methods of self-assembly, with primary emphasis on the novel Non-Volatile Additive Solvent Annealing (NVASA) process. Additionally, the copolymer matrix was doped and coated with multiple nanofillers to increase its oil separation efficiency, chemical, thermal, and mechanical stability. Fabricated membranes were tested using synthetic oily water and real-field samples and testing protocols from the oil & gas companies in Qatar. Important parameters we consider in evaluating the membranes performance are water flux and oil rejection, mechanical and chemical durability, cleaning and reuse, and the scalability of the fabrication process. This work will highlight the success of the academic/industrial collaboration between QU, University of Southern Mississippi, University of Houston, and Qatar Shell and ConocoPhillips companies. Our work has been funded by multiple grants from the Qatar National Research Fund (a member of Qatar Foundation).



Example of morphology of PS-b-PEO BCP membranes made using the NVASA process and different swelling ratios of the chloronaphthalene high boiling solvent.

DRINIKING WATER MERCURY CONTAMINATION: CAUSES AND TREATMENT

Alexandra E. Spyropoulou[1], Yannis Lazarou[2], Chrysi Laspidou[1]

aespyropoulou@gmail.com; y.lazarou@inn.demokritos.gr; laspidou@uth.gr

[1] *Civil Engineering Department, University of Thessaly, Greece*

[2] *Institute of Physical Chemistry, NCSR "Demokritos", Greece*

An integrated research was conducted to address the twofold problem of salinization and Hg-contamination in drinking water of Skiathos Island, Greece. The presence of mercury in the water distribution system is attributed to cinnabar deposits in the underlying crustal rock which is effectively mobilized in the presence of chloride ions. The phenomenon appears to follow periods of high-water consumption/pumping during summer and is constantly associated with high chloride ion concentrations, apparently resulting from seawater intrusion into the groundwater. A detailed study of mercury mobilization and speciation in water was carried out under chemical equilibrium conditions by using the PHREEQC program. The groundwater flow model (MODFLOW) was applied to understand the hydrodynamics of the coastal karstic system and the dynamic interaction with the sea. Additionally, for the simulation of the seawater penetration in the karstic aquifer, the SEAWAT code was applied aiming at the introduction of a threshold up to which, the Hg-mobilization will not be triggered. Finally, an innovative low energy membrane process was applied in the laboratory for the treatment of the potable water, revealing that it is possible to achieve simultaneous removal of both Hg^{2+} and salinity, while producing drinking water for human consumption, by combining a low-pressure RO membrane and an MD unit.

***Keywords**: salinization; mercury; treatment, contamination, modeling*

E-waste Derived Zeolite for Heavy Metal Removal from Water

Gordon McKay, Hamish Mackey, Haya Alyasi and Shifa Zuhara
Department of Sustainable Development, College of Science and Engineering,
Hamad Bin Khalifa University, Doha, Qatar.
Email: gmckay@hbku.edu.qa

Abstract

The continuing rise in population has generated the corresponding rise in solid waste in drinking water demand and wastewater produced globally. This study focuses on a process to convert one of the most controversial solid wastes, namely, e-waste printed circuit board, into an ion exchange resin and its application for the removal of heavy metals from wastewaters.

The ion exchange resin is derived from the aluminosilicate component of the PCB by a process called pyrolytic chemical activation which results in upgrading the aluminosilicate to produce an ion exchange resin. This treatment involves using potassium hydroxide, KOH, is used to activate the raw material at 200-250°C at 5°C/min for 3 hours in a muffled furnace in a nitrogen atmosphere. The samples (before and after activation) were also analyzed for the elemental composition, surface area, functionality, using various characterization techniques. These results will only be briefly discussed since they have been reported previously.

The removal of a number of heavy metals from water have been studied and their high exchange capacities on this ion exchange sorbent are presented in terms of their exchange isotherms. The novel ion exchanger has two exchange sites after activation treatment due to calcium ions and potassium ions. During the adsorption studies, in addition to the monitoring of the polluting heavy metal removal by ICP-AES the calcium and potassium ion concentrations were also recorded during the removal of cadmium from the water. Consequently, a novel model was proposed for the binary exchange mechanism with cadmium ions based on using a multistage Langmuir isotherm to identify the different stages of the exchange removal process.

Highlights

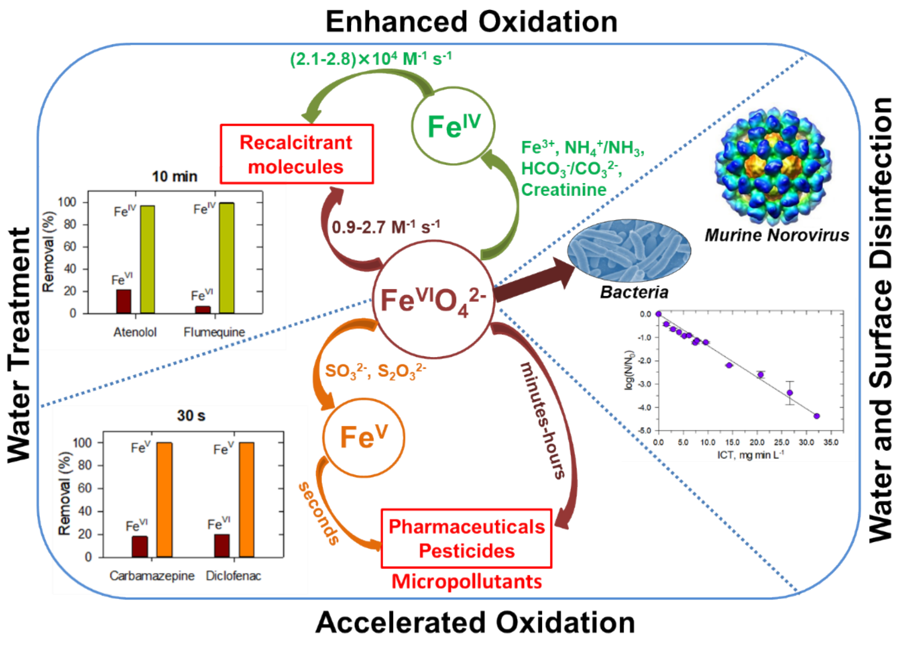
Ion exchange product from e-waste PCB
High exchange capacity for heavy metals removal from water
Novel binary site ion-heavy metal ion exchange model

ENHANCING WATER SUSTAINABILITY BY ACTIVATING FERRATE(VI): ROLE OF HIGH-VALENT IRON INTERMEDIATES

Virender K. Sharma

Program for the Environment and Sustainability,
Department of Environmental and Occupational Health, School of Public Health,
Texas A&M University, College Station, Texas, USA.
E-mail: vsharma@tamu.edu

Iron in +6 oxidation state, called ferrate(VI) ($Fe^{VI}O_4^{2-}$), is an emerging environmentally-friendly sustainable green material, which can play important role in processes like oxygen generation from water, synthesis of organic molecules with selectivity, and treatment of water and wastewater. The theme of the presentation will be to elucidate multi-modal actions of ferrate(VI) in water sustainability by carrying out simultaneously disinfection, coagulation, and oxidation [1]. Examples of disinfecting include inactivation of chlorine resistant microorganisms and coagulation of toxic metals such as arsenic and lead. Oxidative transformation of pharmaceuticals like antibiotics in water will be presented [2]. Recent research on “Activated Ferrate” to oxidize recalcitrant pollutants in water will be discussed. A wide range of micropollutants in water can be degraded by “Activated Ferrate” with high efficiency, in seconds, which would otherwise take several minutes or hours by ferrate(VI) without activation [3]. Advances made in applying different strategies to produce “Activated Ferrate” to achieve enhanced water sustainability will also be presented. Finally, the oxidative mechanisms of “Activated Ferrate” involving highly reactive iron intermediates (i.e., Fe^{V} and Fe^{IV}) will be delineated [4,5]. Overall, iron-based cost-effective material can improve population health by water reuse.



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FABRICATION AND TESTING OF FUNCTIONALIZED GRAPHENE OXIDE-POLYSULFONE MIXED MATRIX MEMBRANES FOR EFFICIENT TREATMENT OF OILY WASTEWATER STREAMS

Omnya Abdalla,[1] **Ahmed Abdala**[2*]

[1]*Gulf Organization for Research and Development, Qatar Science and Technology Park, Doha, Qatar*

[2]*Chemical Engineering Department, Texas A&M University at Qatar, Doha, Qatar*

[*]*Email: ahmed.abdala@qatar.tamu.edu*

Proper treatment of oily wastewater streams can constitute a reusable water source. Membrane technology can provide an efficient treatment process to reduce the content of oil in water streams to an acceptable level. Current commercial polymeric membranes combine ease of fabrication and separation efficiency but suffer from bio and organic fouling. In this presentation, we discuss the design, fabrication, characterization, and testing of ultrafiltration (UF) mixed matrix membranes (MMM) for water oil separation by incorporation of small concentrations of functionalized graphene materials (f-GO) into polysulfone (PS) matrix. The f-GO is synthesized by functionalizing graphene oxide (GO) with amine and carboxylic groups and the functionalization was confirmed by Raman, XRD, and XPS. Subsequently, the PS-f-GO MMMs containing 0, 0.05, 0.1, 0.2, 0.4, and 0.8 wt% of f-GO were fabricated via phase inversion process. The fabricated membrane showed enhanced hydrophilicity and mechanical properties compared to the pristine PS membrane. The loading of f-GO in the MMMs was found to dictate the membrane hydrophilicity, porosity, surface roughness, and separation performance and membranes with low f-GO loading demonstrated improved water flux, oil rejection, and biofouling resistance relative to the pristine PS membrane with an optimum f-GO concentration of 0.1 - 0.2 wt%. This low optimum concertation of f-GO does not impact the cost of the membrane nor the rheological properties of the f-GO-PS solution and therefore does not require alteration of the current commercial fabrication process. In conclusion, our results indicate MMMs based on functionalized graphene are very promising for water oil separation and can serve as the basis of advanced treatment of oil-wastewater streams.

Keywords: water-oil separation, mixed matrix membranes, functionalized graphene oxide, and polysulfone.

Governing with mounting supply risks: Revising the notion of security within the water-energy-food nexus in the Gulf

Mohammad Al-Saidi[1]

Policy, planning and development program, International Affairs Department, College of Arts and Sciences, Doha, Qatar
Email: malsaidi@qu.edu.qa

The water, energy and food supply systems in the Gulf Cooperation Council (GCC) region are coupled through large-scale co-production plants, introduction of renewables, large footprints of resource use and mega-projects. The rapid economic and demographic growth patterns represent major challenges for supply systems. Together, with climate change as an overarching external pressure, the supply infrastructure in the region is undergoing major reconstructions in an effort to expand, modernize and secure resource supplies. Investments in renewables for desalination, energy efficient water production systems, water reuse, alternative food production systems are growing across the region. In this regard, the underlying resource security notion relates to achieving reliable (self)supply and maintaining a high level of sector performance. Such (traditional) notions of security are being challenged through crises such as the COVID-19 pandemic or the Ukrain war. They also neglect key aspects to tackle underlying resource use challenges such as increasing risks related to coupling of systems, dependency of technology and vulnerability to climatic pressures as well as non-environmental risks. In this contribution, alternative notions of security will be explored in terms of their suitability to enrich the sustainability and development debate in the region. Using recent crises and insights on resilience based understanding of resource security, this contribution will outline implications for nexus grovernance in the GCC region, and the wider Middle East.

HYDROGEN PRODUCTION THROUGH SEAWATER ELECTROLYSIS

Ahmed Badreldin[1], Dharmesh Kumar[2], Karim Youssef[2], and Ahmed Abdel-Wahab[1]

[1]Chemical Engineering Program, Texas A&M University at Qatar, P.O. 23874, Doha, Qatar

[2]Qatar Shell Research and Technology Centre, P.O. Box 3747 Doha, Qatar

ahmed.badreldin@qatar.tamu.edu

Green hydrogen (H_2) production through water electrolysis using electricity generated from renewable energy sources presents an opportunity for both developed and developing economies to diversify their energy mix and reduce greenhouse gas emissions. It is also a promising approach for storing intermittent renewable energy sources, such as solar and wind, or through chemical hydrogen carriers such as ammonia for value-added petrochemicals such as fertilizers. However, the current reliance on highly purified buffered fresh water as the feed electrolyte poses a challenge for advancements in green hydrogen production, especially in arid regions facing fresh water scarcity. Nonetheless, the majority of arid countries have access to abundant seawater, which would be a reliable water source if it can be used efficiently and cost-effectively for green hydrogen production. To this end, direct seawater electrolysis (DSWE) has witnessed growing research interest in recent years. Unfortunately, in the complex composition of seawater poses several technical challenges if directly implemented with contemporary industrial electrolyzers. For instance, undesired and kinetically facile chlorine evolution reaction (CER) competes with the desired oxygen (O_2) evolution reaction (OER) at the anode due to the high concentration of chloride present in seawater. CER products are toxic, corrosive, and involve separation costs and environmental impact if discharged back to the sea. Furthermore, precipitable cationic species in seawater, such as magnesium (Mg) and calcium (Ca), tend to easily precipitate due to the local high pH environment near the cathode – thereby deactivating catalytic active sites, and fouling and degrading the cell membrane dividers. pH-Neutral seawater electrolysis offers many advantages over conventional alkaline conditions such as use of earth-abundant electrocatalysts and inexpensive electrolyzer components, inherently safer and environmentally benign operation, and preclusion of Mg and Ca solids precipitation. Despite these advantages, the kinetics of H_2 evolution reaction (HER) and OER are sluggish at neutral pH due to the requirement of an additional water dissociation step, which requires higher overpotentials to achieve the same production rate.

In our work, we address both cathodic and anodic challenges of DSWE through designing electrocatalysts with high stabilities against chloride-induced corrosion, selective anodes towards OER, earth-abundant compositions, and highly-active and stable performance in near-neutral pH operation. We investigate several routes towards suppressing undesired CER at the anode, such as intrinsically OER selective surfaces, chloride suppressing inert anodic overlayers, and interlayers that support polyanionic electrostatic shielding from incoming chloride content. We have strategically designed catalytic surfaces capable of overcoming the thermodynamically limiting water dissociation step during near-neutral pH electrolysis via an anisotropic catalyst design. We achieved this through electronically localized surfaces with heterointerfaced neighboring sites of both high hydrogen (HBE) and hydroxide binding energies (OHBE) for water dissociation, and optimized HBE and OHBE for HER and OER intermediates propagation, respectively. We used textural, surface chemistry, and electrochemical technique to characterize the intrinsic properties and performance of the developed catalysts. Results of these analysis showed that the developed cathodic and anodic materials have very high performance towards near-neutral pH HER and OER, respectively, with strong resistance against chloride-induced deactivation and. This study was made possible by a grant from the Qatar National Research Fund under its NPRP award number NPRP12S-0131-190024, and by Qatar Shell Research and Technology Center.

PILOT TESTING OF ADVANCED MED TECHNOLGY FOR SEAWATER DESALINATION AND BRINE TREATMENT

Abdel-Nasser Mabrouk,[1,2] **Jasir Jawad,**[1] **Simjo Simson**[2]

[1] *Water Center, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, 34110, Doha, Qatar.*

[2] *College of Science and Engineering, Hamad Bin Khalifa University, 34110, Doha, Qatar.*

Corresponding Author: Dr. Abdelnasser Mabrouk, email: aaboukhlewa@hbku.edu.qa

Abstract

Water is the number one resource for economies, and desalination is a key technology to produce sufficient and affordable drinking water. Desalination is the key sustainable solution and provides **97%** of water needs in Qatar. The site-specific and unique Gulf seawater characteristics have influenced the selection of the suitable desalination technology and lead to the exercise of compromise between the thermal and membrane desalination. There are many factors such as energy efficiency, reliability under harsh conditions, and lower unit costs. Due to the characteristics of harsh Gulf seawater (high temperature reaching more than 37 °C in summer, residuals of boron, high TDS and bromides, and the severe fluctuations in the seawater intake quality), the RO membrane technology facing a true operational challenge. When it comes to the water security, the reliability and durability are among the important parameters of selecting suitable desalination technology. Accordingly, thermal desalination is still considered a reliable technology, however, its typical specific energy consumption showed that a significant potential for improvement compared with the thermodynamic limits of separation of 1.0 kWh/m^3. Environmental impact of huge brine discharge to the sea from desalination plants also one main motivation of this project.

This work presents a novel integration of Multi Effect Distillation with Absorption compressor (MED-AB) to reduce the energy consumption and unit water cost. The MED-AB pilot plant has been installed with a nominal capacity of 25 m^3/day to validate the concept under a seawater salinity of 57,500 ppm (West of Qatar). Both pilot testing and the simulation results confirm the features of the novel design of the MED-AB process. Simulation of a commercial evaporator of 15 MIGD capacity showed that the specific energy consumption of the proposed MED-AB is calculated as 4.8 kWh/m^3, which is 60% lower than the existing MED-TVC plant (13 kWh/m^3). Compared to the traditional MED-TVC, the seawater feed and pumping power of MED-AB process is lower by 70% and 55%, respectively. The results confirm the minimization of the environmental impact of dumping thermal energy back into the sea and reduces the plant's capital investment, covering feed pumps size and the intake/outfall civil work. The levelized unit water cost of the MED-AB is calculated as 0.46 \$/m^3, which is 22% lower than that of a conventional MED-TVC desalination plant. The novel MED-AB technology would create a potential solution for the industrial applications of high salinity byproduct and solar desalination.

PRESSURE-RETARDED OSMOSIS APPLICATION TO PRODUCED WATER FROM THE OIL & GAS INDUSTRY

Dareen Dardor[1], Mashael Al Maas[1], Joel Minier-Matar[1],
Ahmed Abdel-Wahab[2], Ho Kyong Shon[3], Samer Adham[1]

[1]ConocoPhillips Global Water Sustainability Center, Doha, Qatar
[2] Chemical Engineering Program, Texas A&M University at Qatar, Doha, Qatar
[3] Center for Technology in Water and Wastewater, University of Technology Sydney, Australia

Abstract

Pressure-retarded osmosis (PRO) is a promising membrane technology for harnessing the osmotic energy of saline solutions. PRO is typically considered with seawater/river water pairings however greater energy can be recovered from hypersaline solutions including produced water (PW) from the petroleum industry. One of the major challenges facing the utilization of hypersaline PW is its high fouling propensity on membranes. In this unique experimental evaluation, real PW from different sites was pretreated to varying degrees: i) minimal, ii) intermediate, and iii) extensive. The treated effluent was subsequently used for PRO testing and fouling rates were assessed for different membrane configurations over multiple cycles. Commercial grade flat sheet (FLS) coupons and novel hollow fiber (HF) modules were compared to validate the lower fouling propensity of HF membranes in PRO application. When minimally pretreated PW (10-micron cartidge filtration (CF)) was tested in FLS mode, severe membrane fouling occurred and the PRO flux decreased by 60%. In contrast, HF modules showed <1% flux decrease under both minimal and intermediate pretreatment schemes. Extensive pretreatment (1-micron CF, dissolved air flotation (DAF), powdered activated carbon, and microfiltration) reduced FLS PRO flux decline to <1%. These results confirm that PW can be treated to suitable levels for PRO application to avoid membrane fouling. Further validation of these pretreatment methods requires long term pilot testing and techno-economic assessment.

Keywords: Hypersaline produced water, pressure-retarded osmosis, pretreatment, membrane configuration, oil & gas industry, energy generation.

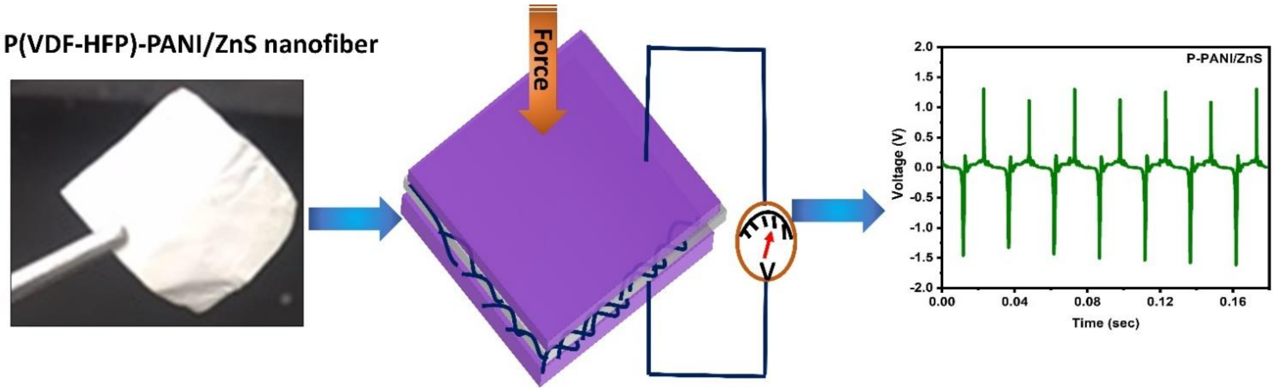
SELF-POWERED FLEXIBLE NANOCOMPOSITE FIBERS FOR PIEZOELECTRIC ENERGY HARVESTING APPLICATIONS

Hemalatha Parangusan, Jolly Bhadra*, Zubair Ahmed, Noora Al-Thani

Qatar University Young Scientist Centre (QUYSC), Qatar University, P.O. Box 2713 Doha, Qatar.

**Email-jollybhadra@qu.edu.qa*

Recently, the use of piezoelectric nanaogenerators to scavenge energy from the environment and convert it to electrical energy has received a lot of attention as a renewable energy source. Piezoelectric materials can convert mechanical energy into electrical energy and thus find application in wearable and portable electronic devices [1]. The present work aims to develop flexible electrospun composite fibers for designing self-powering nanogenerator. The co-polymer of [P(VDF-HFP)] is used as the base polymer and the PANI/ZnS core-shell microsphere is used as the filler reinforcement. The [P(VDF-HFP)]/ PANI/ZnS electrospun nanofibers are prepared by electrospinning technique. This technique helps in the alignment of polymer dipoles in specified directions, resulting in remarkable piezoelectric properties in the resultant fibers. The study reveals that the crystallinity structure of the composite has improved, leading to increased piezoelectricity. It also demonstrates that the composite's dielectric constant has improved, indicating that the developed material's storage capabilities have improved. The enhanced piezoelectric properties is due to β-phase fraction, alignment of polymer dipole moment, filler dispersion, filler alignment and the interfacial interaction between the polymer chains and the PANI/ZnS particles. This enhancement in the piezoelectric properties reflects the ability of these composite films in constructing piezoelectric nano devices with higher efficiency. In addition, the nanocomposite displays high dielectric constant and making it suitable for energy storage applications.



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TREATMENT AND REUSE OF WASTEWATER IN GCC COUNTRIES: PROSPECTS AND OPPORTUNITIES

Moza Alkaabi, Noura Boudjema, Fatema Alshowaikh, Haleema Saleem, Syed Javaid Zaidi*

*UNESCO Chair for Desalination and Water Treatment,
Center for Advanced Materials (CAM), Qatar University, Qatar
E-mail address: szaidi@qu.edu.qa

Abstract

The scarcity of freshwater has developed to be a global challenge, and this has resulted in the production of fresh water from wastewater. Several nations across the globe carry out the discharge of the wastewater to the surroundings, and this wastewater can cause several harmful effects to the earth and the living beings. The term 'wastewater' refers to the discharge of sewage, storm water, water emissions from factory etc. The endless commitment for defending the surroundings as well as its inhabitants from the contamination of wastewater has resulted in a substantial improvement in the techniques for wastewater treatment (WWT). The current study focuses on studying the potential risks as well as benefits associated with the use of treated wastewater along with analyzing the GCC regulations related to wastewater reusing. Moreover, various WWT techniques and different reuse processes/technologies were discussed, and several former research works executed across the GCC countries in this field were assessed. The treatment of wastewater demonstrates several advantages like it helps in lowering the pollution of environment and help countries with restricted access to clean water, to meet their requirements. Techniques for the treatment of wastewater such as biological treatment, coagulation-flocculation, and different membrane technologies have been studied. Adequate wastewater management demonstrates higher possibility for alleviating the clean water scarcity in the GCC countries [1]. The treated wastewater has been noted to have extensive applications in construction, domestic, and agriculture sectors. Each GCC country has distinct policy as regards the management of wastewater. And additional studies must be carried out as the GCC territory is competing for producing new WWT plants to accommodate their increasing requirements for clean water.

Acknowledgements

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Reference

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Water, Energy, Food, and Circular Economy

Rabi Mohtar, Texas A&M University, American University of Beirut

Presentation for the American Chemical Society, Doha Chapter Symposium on Sustainability

The primary resources of water, energy, food, and health are threatened by the growing gap between demand and supply. Population growth, demographic changes, climate change, and changes in land use are each threatening the sustainability of these primary resources. Their interconnected nature and tight coupling further complicate the gap of these resources. This system of systems is threatened, and this threat constitutes one of the major challenges of the 21st century.

The presentation outlines the water-energy-food-health nexus as an emerging discipline and a platform for improved management of our primary resources for future generations. It includes the history and evolution of the nexus concept over the past twenty years and its transition from a classroom exercise to a full-fledged discipline with modeling, data, and real-life applications. We will define the nexus and provide a working definition around this emerging discipline. We will share success stories and applications of the nexus in various hotspots around the world in the hope of presenting some of the applications that have evolved over the last decade. We will also share some trends and future opportunities in nexus applications, particularly highlighting the circularity of the food and agriculture system as one of these applications that must be considered in terms of the stresses upon agriculture regarding its ability to access water and energy and the increasing demand for food and food security as a highlight of the coming challenges. We will then offer some conclusions from the ongoing research and current activities.

Natural Gas Processing

A PROCESS CONCEPT FOR DIRECT METHANE CONVERSION TO CHEMICALS THROUGH SYNERGY INTEGRATING OF OCM AND MDA REACTIONS

Anchu Ashok[1], Izabel MEDEIROS COSTA[2] ,Ma'moun Al-Rawashdeh[1]*
1. Department of Chemical Engineering, Texas A&M University at Qatar, Doha, Qatar
2. TotalEnergies One Tech Belgium, Parc Industriel de Feluy C, 7181 Seneffe, Belgium
**Corresponding author: mamoun.al-rawashdeh@qatar.tamu.edu*

One of the major challenges in the field of the natural gas industry is the conversion of methane into more value-added products in a sustainable and economical way[1]. Oxidative coupling of methane (OCM) and methane de-hydroaromatization (MDA) are two promising direct routes of methane conversion to basic chemicals that received wide attention in recent years. MDA reaction is a one-step reaction that converts methane into valuable aromatics and hydrogen with zero CO_2 emission from the reaction stoichiometry [2]. OCM reaction is a one-step reaction that converts methane in the presence of an oxidant, typically oxygen into valuable C_2+ products such as C_2H_4 and C_2H_6 along with CO_2 as a main product [3]. Although very attractive reactions, they are not yet commercialized due to certain challenges such as fast catalyst deactivation in MDA, highly endothermic reaction, and thermodynamic limitations which limit the maximum conversion. OCM, on the other hand, is highly exothermic which requires strict and difficult heat management, and has a tradeoff between selectivity for higher hydrocarbons and methane conversion. Several approaches have been explored to recover the MDA catalyst activity to address the challenge of fast deactivation. This includes adding different regenerating molecules such as H_2, for reductive regeneration, and or CO_2 or O_2 for oxidative regeneration. The other option is through adjusting the feeding mode and timing of introducing these regenerating molecules as pulse, periodic, or co-feeding. This study aims to address some of the mentioned technical challenges by possible integration options between exothermic OCM and endothermic MDA reaction. Heat integration is the first potential advantage from this coupling which can reduce the external heating or cooling resources needed for both reactions which would significantly decrease the overall process CO2 emission, and help in strict heat management. Another option is mass integration which can be accomplished by directing the OCM reaction outlet to be the feed for the MDA catalyst. This in-situ generation of the reactive regeneration molecules from the OCM reaction can help stabilize and MDA reaction and possibly boost the benzene selectivity because of ethylene addition to the MDA catalyst. In this study, we explore the option of mass integration by combining OCM and MDA catalysts in the same fixed bed reactor. The exothermic $MnWNa/Al_2O_3$ catalyst was placed above the endothermic Mo/HZSM catalysts with a separation of quartz wool in between. Various parameters are accounted for in this study that including the amount of catalyst, feed ratio, stacking strategy, gas flow rates, sequence of adding regenerating molecules. The initial outcomes from this ongoing experimental investigation will be presented along with opportunities and limitations toward the development of this promising process concept.

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CARGEN™: A NOVEL CO_2 UTILIZATION TECHNOLOGY FOR THE SYNERGISTIC CO-PRODUCTION OF SYNGAS AND CARBON NANOTUBES

Challiwala, Mohamed Sufiyan[1,2,4]; Choudhury, Hanif Ahmed[2,4]; Sengupta, Debalina[1,4]; El-Halwagi, Mahmoud M.[1,4]; Elbashir, Nimir[2, 3, 4 *]
[1]*Artie Mc Ferrin Department of Chemical Engineering, Texas A&M University, TX, USA*
[2]*Chemical Engineering Program, Texas A&M University at Qatar, PO Box 23874, Doha, Qatar*
[3]*Petroleum Engineering Program, Texas A&M University at Qatar, PO Box 23874, Doha, Qatar*
[4]*TEES Gas & Fuels Research Centre (GFRC), College Station, TX, USA*
Email: nelbashir@ tamu.edu

Motivated by the global climate change concern and the greenhouse gas (GHG) emission challenge, the novel CARGEN™ technology is designed, experimentally proven, and scaled-up to decarbonize the carbon emissions from the process industry. CARGEN™ is built to address the process challenges of dry reforming of methane (DRM), which is an attractive route to convert CO_2 and CH_4 to syngas. Catalyst deactivation via carbon formation due to selective surface carbon forming side reactions in DRM is understood to be its primary challenge alongside secondary and tertiary challenges like high endothermicity and downstream incompatible syngas ratio. CARGEN™ technology comprises of a system of two-reactors that is designed based on a multidisciplinary approach that utilizes concepts of Chemistry, Catalysis, and Process Systems Engineering to systematically and step-wise address DRM challenges. CARGEN™ shifts the reaction chemistry by taking advantage of product selectivity at different operating conditions to produce carbon nanotubes in first reactor and a tunable syngas in the second reactor. The synergism in energetics of the CARGEN™ concept allows for a significant reduction in the energy requirement compared to the conventional reforming processes. CARGEN™ technology has demonstrated at least 65% CO_2 conversion to high value carbon nanotubes while delivering syngas quality that meets gas-to-liquid (GTL) industry requirements. Moreover, CARGEN™ technology can also be configured to produce hydrogen. A CO_2 life cycle assessment (LCA) of the CARGEN™ technology indicates at least 40% reduction in the carbon footprint compared to the state-of-the-art natural gas reforming technologies. CARGEN™ concept was initially tested at tens of milligram scale in Thermogravimetric Analysis (TGA) equipment and then scaled-up to multi-grams and finally to kilo-grams scale of production in custom-made and in-house designed reaction setups. The nanotubes produced from CARGEN™ process have been tested using SEM, TEM, TGA-oxidation, and RAMAN analysis, and have found to be consistent in quality that is comparable to commercially available nanotubes. Specifically, in terms of the Differential Thermogravimetric Assessment (DTA) study, the CARGEN™ produced CNTs compares with the commercial quality nanotubes. In terms of RAMAN analysis, the I_D/I_G, $I_G/I_{G'}$, and the $I_D/I_{G'}$ ratio of CARGEN™ produced CNTs was less than commercial quality nanotubes, implying that the CARGEN™ nanotubes are of better quality and have less distortion compared to commercial quality nanotubes. Moreover, a techno-economics assessment of the CARGEN™ process revealed an attractive profitability when scaled-up to commercial scale unit. This presentation will highlight the unique scale-up journey of the technology while discussing the merits for CO_2 conversion and industrial decarbonization. This work was a part of a mega-project (NPRP-X 100-2-024), and Responsive Research Seed Grant (RRSG 2021).

DEVELOPMENT OF HIGHLY STABLE SINGLE-SITE METAL ZEOLITES AND NEW TRENDS FOR THEIR APPLICATION IN METHANE CONVERSION

Izabel C. Medeiros-Costa[1*], Hugo Cruchade[2], Florent Dubray[2], Stanislav V. Konnov[2], Jean-Pierre Gilson[2], Julien Grand[1], Jean-Pierre Dath[1], Nikolai Nesterenko[1], Olivier Miserque[1], Svetlana Mintova[2]
[1]Total One Tech Belgium, Feluy, B-7181 Seneffe, Belgium.
[2]Normandie Université, ENSICAEN, UNICAEN, CNRS, Laboratoire Catalyse et Spectrochimie (LCS), 14050 Caen, France.

Corresponding author: izabel.medeiros-costa@totalenergies.com

The development of catalysts with high stability is an important step towards the valorization of methane into valuable chemicals. More specifically, methane dehydroaromatization (MDA) requires catalysts that withstand high temperatures and whose active sites remain stable over time on stream. To respond to this challenge, we developed defect-free MFI crystals through the incorporation of single-site framework Mo atoms. The incorporation of Mo occurs through a simple post-synthesis hydrothermal treatment under mild temperatures. Such treatment proved to be effective in inserting Mo into both pure-silica and Al-containing MFI, while healing the silanol defects present in the parent zeolitic structure. The result is a zeolitic-based catalyst with a perfect structure, which provides superior thermal and catalytic stability.[1] The quality of the zeolitic crystals after treatment with Mo is remarkable, having previously only been observed in large crystals synthesized with hydrofluoric acid. We also investigated the role of silanols in the incorporation of Mo in the zeolite framework and we were able to identify a specific type of silanols as a gateway to the insertion of Mo atoms in the MFI framework.[2]

The novel single-site Mo-MFI was tested in MDA reaction and its performance in terms of stability was superior to conventional impregnated Mo-MFI containing similar Mo loading.[3] Characterizations performed on the spent catalyst indicate that Mo remains dispersed in the zeolite framework of single-site Mo-MFI even after several catalytic-regeneration cycles at high temperatures, and that the zeolitic crystalline structure is also conserved. On the other hand, in the case of the conventional impregnated Mo-MFI zeolite, a deactivation of the catalyst is observed due to the migration of Mo and formation of the inactive aluminum molybdate, which further confirms the superiority of single-site Mo-MFI. Our recent studies exploring single-site zeolites indicate that the use of different catalytic bed configuration can be beneficial for MDA reaction, notably in the reduction of coke over the Mo-containing active phase.

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GAS-TO-CHEMICALS AS A DECARBONIZATION ENGINE FOR THE DOWNSTREAM INDUSTRY

Nikolay Nesterenko, Sasha Strasser
Sulzer Chemtech, Switzerland
E-mail: Nikolay.Nesterenko@sulzer.com

Natural gas is traditionally seen as a cost advantageous feedstock for chemical production. The utilization of methane for chemical production, often considered as the “Holy grail” of the 21st century, and historically could not economically compete with the traditional petrochemistry due to higher investments costs. In current environment, most probably, there is not an urgent need any more to develop a new on-purpose process to produce fossil olefins or aromatics from natural gas. However, a process helping the downstream industry with CO_2 utilization and with a supply of low carbon hydrogen is highly desired. Moreover, the target for a future technology based on the fossil feedstock should be primarily on a creation of the sustainability value while complementing the economic benefits from a low carbon chemical production.

Among fossil feedstocks, methane shows the highest difference in energy with the chemical intermediates resulting in a significant decarbonization potential of a Gas-to-Chemicals process. The latter also will make these technologies attractive and potentially economically completive with the traditional petrochemistry in near future.

Despite significant investments in renewable energy production, these resources will be remaining in a deficit during the period of the energy transition and its impact should be optimized and magnified. Gas-To-Chemicals is an efficient tool to leverage the decarbonization potential of the renewables. Gas conversion may become a decarbonization engine for the downstream industry and an efficient way for renewable energy valorisation.

Three approaches based on the soft oxidants, electrification, and autothermal co-processing will be discussed. Implementation of the latest innovations from Sulzer based on Br-activation helps unlocking the biogas potential for bio-products manufacturing.

Conversion of CO_2 to CO as a part of a Gas-To-Chemicals plant offers a viable option for CO_2 utilization and a solution for CO_2 circularity inside assets. Methane-to-chemicals complexes also contribute to decarbonization of refinery & petrochemicals complexes via CO_2 avoiding from firing of off-gases and by providing low carbon H_2 to substitute the hydrogen from SMR.

The electrified processes to co-produce in Gas-To-Chemicals hydrogen from methane with chemicals may become particularly attractive due to credits for renewable hydrogen production in the future. The energy requirement for an electrified process for H_2 production is at least twice as lower from methane feedstock in comparison with the state-of-the art water electrolysis while yielding in both cases CO2 - free renewable H_2.

With the most recent technical advances in Br-mediated activation of methane, there are very good prospects to successfully address “The Methane Challenge” while offering a viable solution for decarbonization of the assets.

INTEGRATING LOW CARBON PROCESSES TO UPGRADE METHANE TO PLATFORM CHEMICALS

Muhammad Umar Jamil[a], Other authors

[a]Research Engineer, TotalEnergies Research Center Qatar, Affiliations

muhammad-umar.jamil@external.totalenergies.com

Efficient and sustainable natural gas conversion processes are required for achieving low to zero carbon emissions while producing value added chemicals like ethylene, hydrogen, aromatics, etc. These products play a strategic role for Qatar's economy due to the presence of large amount of feedstock as natural gas reserves. Significant research has been carried out so far in the field of direct methane conversion on oxidative (OCM) and non-oxidative (NOCM) coupling of methane. Various challenges exist for these processes to be commercially viable and are important to be addressed. In this work, we present an overview of integrating OCM and MDA processes and the associated challenges for process intensification in a chemical reactor. While this brings about several advantages like lower carbon emissions, energy, and cost savings, the technical challenges remain. These are not limited to thermal runaways and reactor hotspots, reactor modeling limitations and heat transfer coefficient, catalyst coking, integrated reactor equipment design, optimized operation, control, and safety. These topics are widely interdisciplinary and require collective contribution from the experts of various fields. Endorsing such technologies towards the commercial scale would require working on these topics simultaneously and collaboratively. Thus, can help in understanding the bigger picture and identify the objectives sooner than later.

NUMERICAL DESIGN AND EXPERIMENTAL EVALUATION OF A SOLAR REACTOR FOR THE CATALYTIC DRY REFORMING OF METHANE

Tayseir M. Abd Ellateif*, Konstantinos E. Kakosimos

Chemical Engineering Department, Texas A&M University at Qatar, Doha, Qatar

**Corresponding author e-mail:* k.kakosimos@qatar.tamu.edu

ABSTRACT

Methane dry reforming is a process to produce “syngas” (H_2 and CO) which is a major precursor for many chemicals and ultra-clean fuels. It is also a CO_2 assisted process that leads to the conversion of CO_2 to higher value products and an overall reduction of CO_2 emissions from the chemical industry. For this reason, there is a good number of studies and reviews towards improving the process efficiency, designing new catalysts, and utilizing solar energy. This study is part of a bigger effort that explores novel catalysts and processes for CO_2 conversion, with the goal of achieving processes in which CO_2 input is greater than CO_2 output at any stage, with the ultimate objective of significantly lowering Qatar’s CO_2 footprint. This study focuses on the utilization of solar energy to activate the Atomic Layer Deposition (ALD) based catalyst and drive the dry reforming reaction directly. First, we present the numerical design of a lab scale solar tubular reactor and second, the experimental evaluation of the reactor and dry-reforming reaction conversion efficiencies.

The thermal and optical performance of a solar tubular reactor/receiver depends upon the geometry of the receiver, optical and thermophysical properties of a receiver’s material and reaction conditions. Initially, out 7kW high flux solar simulator (HFSS) is modeled using a commercial software, TracePro®, to obtain the intensity and distribution of the incident radiation flux. The tubular receiver has an internal diameter of 20 mm and an “active” length of 20 mm. To achieve the maximum possible optical efficiency and homogenous heating of the receiver a novel cavity is designed which reflects and focuses the incident flux on the tubular receiver. Multiple scenarios were investigated and optimum results are presented here. Following the solar reactor manufacturing, an experimental setup was fabricated to study the performance of the proposed catalysts under simulated on-sun conditions. Commercial catalyst (20% Ni/Al_2O_3) has been used in a fixed bed configuration (0.2 g catalyst premixed with 2 g of inert quartz). The gas mixture (CH_4, CO_2, Ar, He with 5%: 5%: 2%: 88%) was fed into the reactor at weight hourly space velocities (WHSV) in the range of flow 2,000 ml/min/g to 10,000 ml/min/g. The catalytic bed was directly irradiated with a high flux solar simulator using 1-3 Xe arc lamp (6 kW each) producing three different temperature levels (550 ^{o}C, 650 ^{o}C and 800 ^{o}C). Herein we report the methane reforming conversion efficiencies and catalysts’ activities. Moreover, the morphological, chemical, and stability changes of the catalytic particles have been studied and reported here.

Keywords: Solar simulator, methane, dry reforming, catalytic reactor.

PREDICTION OF ADSORPTION AND DIFFUSION OF SHALE GAS IN HYBRID PORES CONSISTING OF KAOLINITE AND KEROGEN USING MOLECULAR SIMULATION

Noura Dawass,[1] **Manolis Vasiliadis**,[2] **Loukas D. Peristeras**,[2] **Konstantinos D. Papavasileiou**,[2]
Ioannis G. Economou[1]

[1]*Chemical Engineering Program, Texas A&M University at Qatar, Education City, Doha PO Box 23874, Qatar*
[2]*Molecular Thermodynamics and Modelling of Materials Laboratory, Institute of Nanoscience and Nanotechnology, National Center for Scientific Research "Demokritos", GR-15310 Aghia Paraskevi, Attikis, Greece*
E-mail: noura.dawass@qatar.tamu.edu

As the world's energy demand is rising and conventional energy resources are draining, shale gas is becoming increasingly important in mitigating the difference between supply and demand. While technologies such as horizontal drilling and hydraulic fracturing are currently used, the production of shale gas is still considered challenging [1]. This is partly due to the lack of knowledge about the behaviour of fluids in such formations, as well as the lack of understanding of gas adsorption and transport mechanisms. In this respect, molecular simulation is a powerful tool that can address molecular interactions between molecules and pore surfaces. Accounting for the effect of confinement is especially important in the case of shale gas as they are trapped in micro- and nano-sized pores [2]. Thus far, most computational studies have focused on studying shale gas in a single type of porous media consisting of either clay/inorganic material (e.g. montmorillonite, kaolinite, illite) or organic matter (kerogen) [2]. In this study, we investigate the behaviour of shale gas in structures comprised of kerogen [3] (organic) embedded between two kaolinite (clay) walls [4], and with slit pores introduced between one of the clay walls and kerogen (Figure 1). Initially a robust methodology for the construction of hybrid pores is presented. The behaviour of the structures in terms of their mechanical stability is investigated. Secondly, we report the thermodynamic and transport properties of methane, ethane and a CH_4, C_2H_6, N_2, CO_2 mixture with a composition resembling that of shale gas in different hybrid pores widths at standard temperature and two pressures. The amounts of fluid adsorbed are computed by employing iterative steps of Grand Canonical Monte Carlo (GCMC) and Molecular Dynamics (MD) simulations. Additionally, MD simulations in the NPT ensemble are performed to compute density profiles and diffusion coefficients.

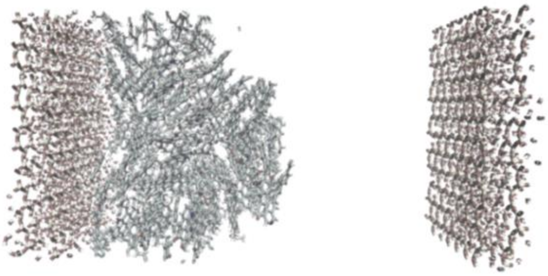

Figure 1. A schematic representation of a hybrid pore consisting of kaolinite walls, kerogen and a slit pore.

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QATAR MOVING TOWARDS A NET-ZERO EMISSION: CARBON MANAGEMENT AND CLIMATE CHANGE SOLUTION

***Abdulkarem Amhamed and Ahmed Sodiq**

Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Qatar Foundation, Doha, Qatar.
Aamhamed@hbku.edu.qa

As the concentration of carbon dioxide (CO_2) in the atmosphere continues to rise, and the reality of global warming challenges hits the world, policymakers and global research societies are racing to address climate change challenges brought about by high atmospheric concentration of CO_2. There are several available options for CO_2 emissions reduction in the atmosphere. However, retrofitting CO_2 capture facility to some industrial plants is difficult, because old plants were constructed with no CO_2 capture systems in mind. Even with available CO_2 capture facility onsite, most plants can only capture their emissions in the range of 50-94%, the uncaptured CO_2 apparently finds its way into the atmosphere. Even in an ideal industrial setup, in which 100% of CO_2 generated is captured onsite, it is still technically difficult to directly apply end-of-pipe capture system to the CO_2 emitted by transport sector (i.e., marine, aviation and land transports), which contributes about 50% to global greenhouse gas (GHG) emissions. As a result, we must create ways to return the atmospheric concentration of CO_2 to the pre-industrial era, or find means to reduce its impacts on humans/environment in a way that is independent of CO_2 generation origin. Returning the atmospheric concentration of CO_2 to the pre-industrial era is almost impossible to achieve in this century, but keeping the global warming at ~1.5 °C more than the pre-industrial era is possible but would involve adoption of aggressive carbon dioxide removal (CDR) technologies, which must ensure the removal of between 100 and 1000 $GtCO_2$ by the year 2100. Among all the current CDR technologies, direct air capture (DAC) is the likely technique to deliver the needed CO_2 removal because it is independent of CO_2 emission origin, and the capture machine can be stationed anywhere, especially in a location where the price of energy is very cheap or where renewable energy is relatively abundant.

In this presentation, I will be highlighting the global and Qatari efforts in CO_2 mitigation strategies and the objectives of CO_2 cluster program in Qatar, which involve the integration of DAC with the traditional HVAC systems, as a preexisting technology, to capture CO_2 directly from the atmosphere.

STRATEGIES FOR CO_2 CAPTURE, UTILIZATION AND STORAGE (CCUS)

Muhammad Umar Jamil[a], Other authors

[a]Research Engineer, TotalEnergies Research Center Qatar, Affiliations

muhammad-umar.jamil@external.totalenergies.com

Energy transition is taking place globally for achieving the net zero target by 2050. Scientific focus has shifted towards cleaner energy, less emissions and sustainable production. In this regard, Carbon Capture Utilization and Storage (CCUS) can play a significant role. Although maturing, the carbon utilization start-ups around the world are focusing on a variety of products. Amongst which, carbonates produced via carbon mineralization are of key interest from the utilization as well as permanent storage point-of-view. However, the challenge widely remains on the availability of a high amount of CO_2 being emitted versus the potential of the available technologies. Hereby, we present an overview and analysis of the current carbon mineralization startups. These results can provide pathways for understanding the opportunities and challenges in the field of carbon management and pave the direction towards achieving the sustainable development goals.

SUSTAINABLE ENERGY CARRIERS FROM NATURAL GAS FOR OVERSEAS ENERGY TRANSPORT

Yusuf Bicer

Division of Sustainable Development, College of Science and Engineering, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar
E-mail: ybicer@hbku.edu.qa

There is an increasing motivation to transit from heavy carbon fuels to low carbon or carbon-free fuels especially considering the adverse effects of climate change. Moreover, existing fossil fuel resources are not evenly distributed worldwide, causing an energy imbalance in supply and demand. Therefore, there is a need to transfer energy effectively from energy-producing countries to energy-consuming countries. Long-distance energy transfer is commonly done by liquefied natural gas (LNG) via ocean tankers. However, due to the carbon-containing nature of natural gas, other energy carriers have become potential replacements. In this regard, sustainable energy carriers such as hydrogen, ammonia, methanol and dimethyl ether (DME) emerge as possible solutions. In this study, a comparative life cycle assessment of sustainable energy carriers produced from natural gas or renewables is conducted to investigate the emissions generated from the complete life cycle phases in which boil-off (BOG) gas phenomena is taken into account. It is essential to estimate the carbon emissions through the complete life cycle of these selected energy carriers, including production, storage, ocean tanker transport, as well as final consumption. Moreover, this study calculates the cost of production and transportation of these energy carriers by accounting for BOG and emitted CO_2 as a unit cost within the total cost. It is noted that BOG losses reduce the quantity of the energy carriers during storage and ocean transportation phases, which directly affects their economic value. The results show that liquid hydrogen produced from solar electrolysis is the cleanest energy carrier (42.50 g CO_2 eq./MJ), followed by liquid ammonia (60.76 g CO_2 eq./MJ) produced from photovoltaic-based electrolysis. Economic analysis results show that when BOG cost is considered, the transportation costs of LNG, liquid ammonia, methanol, DME, and liquid hydrogen produced from natural gas 0.74 $/GJ, 1.09 $/GJ, 0.68 $/GJ, 0.53 $/GJ, and 3.24 $/GJ, respectively. DME and methanol can be more economical compared to LNG to transport the energy of natural gas for the same ship capacity. Including the social cost of carbon (SCC) within the total cost of transporting the energy of natural gas, the transportation cost of liquid ammonia is 1.11 $/GJ. In contrast, LNG transportation cost rises significantly to 1.68 $/GJ at SCC of 137 $/t CO_2 eq. Consequently, liquid ammonia becomes economically favoured compared to LNG.

SYNTHESIS OF NANO-MO/ZEOLITE CATALYSTS AND ITS APPLICATION FOR CATALYTIC METHANE DEHYDROAROMATIZATION WITH DENSITY FUNCTIONAL THEORY STUDY

Najam US Sahar Riyaz[1], Maan O. Al-Ejli[1], Nashaat N. Nassar[2], Abdallah D. Manasrah[2], Amjad M. Shraim[1], Ismail Badran[1*]

[1]*Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University, P.O. Box: 2713, Doha, Qatar*

[2]*Department of Chemical and Petroleum Engineering, University of Calgary, Calgary, Alberta, Canada, T2N 1N4*

Keywords: Nanotechnology, methane dehydroaromatization, methane conversion, liquefied natural gas.

The conversion of methane to value-added hydrocarbons is gaining interest given the current global scenario. The dehydroaromatization of methane (MDA) is becoming increasingly popular as it has the potential to produce clean fuel. In this work, nano-Mo/zeolite catalyst was prepared via the precipitation/hydrothermal method. The chosen synthesis technique allowed surface modifications by using different metals, resulting in enhanced catalytic properties.

Direct nonoxidative methane conversion over the as prepared nano-Mo/zeolite catalyst was studied using a hydrogen permeable tubular membrane reactor. The MDA reaction products were monitored using Gas Chromatography and the formation of hydrogen, ethylene, and small hydrocarbons were observed. Significant improvement in methane conversion was achieved by continuous removal of hydrogen from the membrane reactor by vacuum pump.

The catalytic dehydrogenation of methane on molybdenum oxide (MoO_3) was also studied using periodic density functional theory calculations. Two different supercells were studied using the PBE-D functional. The results showed that adsorption on a smooth surface is preferred by methane. The calculations also allowed for a reaction mechanism for hydrogen formation to be derived in which the first energy barrier was calculated to be 66.4 kJ/mol. This work yielded important results which lay the foundation for future research into the MDA and provided useful insights into the synthesis technique for nanoscale catalysts for this reaction, as well as the effect of transition metal doping on the performance of the nanocatalysts.

ZEOLITE CRYSTAL ENGINEERING - MULTISCALE ASPECTS

Jean-Pierre Gilson[1], Dr. Svetlana Mintova[1], Dr. Valentin Valtchev[2]
[1]ENSICAEN - CNRS, [2]Laboratoire Catalyse et Spectrochimie, Normandie Univ, ENSICAEN, UNICAEN, CNRS
Jean-pierre.gilson@ensicaen.fr

Zeolites are very effective and proven catalysts, adsorbents, ion-exchangers in a multitude of applications in the prodution of fuels, chemicals and many others are emerging in new fields (sensors, medical...). Scientific and industrial progress on these strategic materials is based on two complementary approaches:

i) the discovery of new structures

ii) the science-based adjustment of the properties of existing structures to fit the needs of current or emerging processes. In Caen, this is referred to as "*Zeolite Crystal Engineering*".

Many properties can be controlled by a large number of techniques and a useful way to classify them is by looking at the scales of such modifications, ranging from the (sub)nm, µm to the mm/cm

Some recent examples at these three different levels will be discussed:

1) **sub-nm:** point defects in zeolites (silanols) can be almost eliminated by inserting during or after a nanozeolite synthesis transition metal ions such as W, Mo, V…. These atomically dispersed ions in the zeolite framework are extremely stable and provide interesting properties in natural gas upgrading[1-4]. By treating the FAU zeolite with an unbiased (*i.e.,* the resulting Si/Al of the zeolite is unchanged) leaching agent (eg. NH_4F, NH_4HF_2), hitherto unacessible sodalite cages are opened and available for catalysis[5,6].
2) **µm:** The unbiased leaching of zeolites reveals their mode of synthesis by a stepwise deconstruction of the defect zones in crystals. This procedure also allows to remove transport limitations and increases significantly catalytic performances[7].
3) **mm-cm:** While zeolites are always produced as powders in the laboratory or at industrial scale, their use requires a shaping step to produce technical bodies (extrudates, mm-sized spheres, µm-sized microspheres…); in such a step, a binder is almost always needed to meet the strict requirements of and industrial process (pressure drop, crush and attrition resistance, heat and mass transport, …). The binder is often considered as a diluent supporting the zeolite active phase a bit like an excipient of an active molecule in pharmacology. We show that zeolte and binder may interact and produce new catalytically active sites under appropriate conditions[8,9]. This last step in the formulation of an industrial catalyst should be also considered as part of the *Zeolite Crystal Engineering* toolbox.

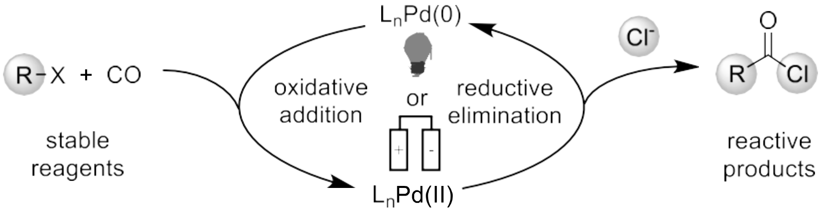
A Life in Chemistry – Remembering Bob Grubbs

ALTERNATIVE ENERGETIC DRIVERS FOR PALLADIUM CATALYZED COUPLING REACTIONS

Bruce A. Arndtsen[1]

[1]Department of Chemistry, McGill University, 801 Sherbrooke St. W., Montreal QC H3A 0B8
Canada
e-mail: bruce.arndtsen@mcgill.ca

The ability of transition metal catalysts to mediate new bond forming reactions has had a dramatic impact on modern molecular synthesis. Nevertheless, a central feature in these reactions is need to balance of often reverse operations on the catalyst so it is regenerated at the end of each cycle of product formation, which can limit catalytic activity and the scope of many transformations. This talk will describe our efforts to address these challenges by introducing alternative, often renewable, energy sources into catalysis, and from this create new bond forming reactions. These include using visible light excitation directly on active palladium catalysts to drive the oxidative addition/reductive elimination cycle in coupling reactions independent of the classical limits in thermal catalysis, or the use of electrochemistry to change the nature of the metal throughout the cycle.[1] Combining these with the favored energetics of carbon monoxide conversion to carboxylic acid derivatives can be used to drive the build-up of reactive products from stable reagents. The use of this chemistry to create ambient temperature and general catalysts for carbonylation reactions, multicomponent transformations, acyl halide or even super-electrophile formation, or new avenues to C-H bond functionalization, will be discussed, as will the mechanistic origins of these influences, and their ability to enable the use of earth abundant catalysts in traditionally precious metal catalyzed reactions.



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Controlled living cascade polymerization to make fully degradable sugar-based polymers

Prof. Tae-Lim Choi

Department of Chemistry, Seoul National University, Seoul, Korea
E-mail: tlc@snu.ac.kr

Monomers derived from glucose, xylose and galactose, which contain an endocyclic alkene (in the sugar ring) and a terminal alkyne, underwent a cascade polymerization to prepare new polymers with the ring-opened sugar incorporated into the polymer backbone. Polymerizations were well-controlled, as demonstrated by a linear increase in molecular weight with monomer-to-initiator ratio and generally narrow molecular weight dispersity values. The living nature of the polymerization was supported by the preparation of a block copolymer from two different sugar-based monomers. The resulting polymers were also fully degradable. They underwent fast and complete depolymerization to small molecules under acidic conditions. Furthermore, by tuning the type of acid-sensitive linkage (hemi-aminal ether, acetal, or ether functional groups), we could change the degradation profile of the polymer and the identity of the resulting degradation products. For instance, the large difference in degradation rates between hemi-aminal ether and ether-based polymers enabled the sequential degradation of a block copolymer.

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DNA NANOSTRUCTURES: DESIGN AND BIOLOGICAL APPLICATIONS

Hanadi Sleiman[1]
[1]*Department of Chemistry, McGill University, 801 Sherbrooke St. W., Montreal, QC H3A0B8, Canada*

DNA nanotechnology can assemble materials on the nanoscale with exceptional predictability and programmability. In a sense, this field has reduced the self-assembly space into a simple ‘language’ composed of four letters (A, T, G, C). Nature, on the other hand, relies on many more supramolecular interactions or ‘languages’ to build its functional structures. Over the last 50 years, supramolecular chemistry has taken advantage of these interactions to assemble materials with highly diverse structures and functions.

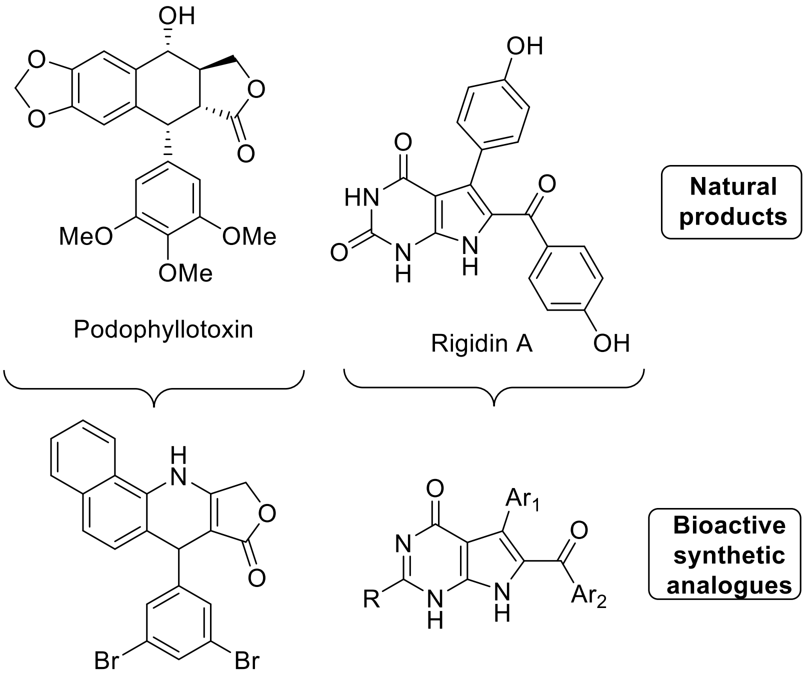
This talk will describe our efforts to merge the field of supramolecular chemistry with DNA nanotechnology. This approach results in new motifs and functionalities that are unavailable with base-pairing alone. Starting from a minimum number of DNA components, we create 3D-DNA host structures, such as cages, nanotubes, and DNA-polymer nanostructures that are promising for targeted drug delivery. These can encapsulate and selectively release drugs and accomplish anisotropic 3D-organization. We find that they resist nuclease degradation, silence gene expression and have a favorable in vivo distribution profile. We will also discuss the ability of small molecules to reprogram the assembly of DNA, away from Watson-Crick base-pairing into new motifs.

FROM METATHESIS & ISOMERIZATIONS TO MULTI-COMPONENT APPROACHES TO BIOLOGICALLY-INSPIRED SMALL MOLECULES

Willem A.L. van Otterlo[1]
[1] Department of Chemistry and Polymer Science, Stellenbosch University, Stellenbosch, 7602, South Africa.
E-mail: wvo@sun.ac.za

This contribution will highlight the **impact of Professor Robert H. Grubbs' seminal research contributions to the field of alkene metathesis** on our earlier research, and then move on to our present focus on our synthesis of bioactive molecules through multi-component reactions.

Small heteroaromatic and benzo-fused molecules have found much application as cytotoxic compounds, particularly in cancer therapy research.[1] In this field, natural products such as podophyllotoxin and rigidin A (see structures below) have been seen as structural muses for novel molecules, as they function by the relatively well understood disruption of the cellular microtubulin assembly required for cell division and thus induce apoptosis.[2]



Generated by way of multi-component reactions

Our research group has in collaborations over the last few years engaged in the area of biologically-inspired organic synthesis (BIOS), specifically to find novel tubulin polymerization modulators. In this talk, approaches concerning the facile synthesis of podophylotoxin [3] and rigidin [4-6] mimics, by way of multi-component reactions, will be reflected on.

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NEW ADVANCES IN POLYMER SYNTHESIS

Craig J. Hawker

University of California, Santa Barbara, CA, 93106, USA

hawker@mrl.ucsb.edu

The orthogonal functionalization of polymeric materials is a critical design strategy for the “bottom-up” fabrication of nanostructured systems. In synthesizing these nanostructures, functional group interconversion, efficient organic transformations and purification of oligomeric building blocks are key to obtaining materials with exceptional properties. The design of discrete and low dispersity building blocks from common polymeric materials and their extension to commercial products will be demonstrated. In addition, a novel methodology for printing 3D objects with spatially resolved mechanical and chemical properties is reported. The power of this approach is showcased through the one-step fabrication of bioinspired soft joints and mechanically reinforced “brick-and-mortar” structures using tailored photochromic dyes.

SYNTHESIS AND APPLICATION OF NOVEL, BICYCLIC ALKYL AMINO CARBENE (BICAAC)-RU LATENT OLEFIN METATHESIS CATALYSTS IN THE DECOMPOSITION OF NON-BIODEGRADABLE POLYMERS

Márton Nagyházi,[1] Gábor Turczel,[1] Robert Tuba[1]

[1]*Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar tudósok körútja 2., 1519 Budapest, P.O. Box 286. Hungary*

tuba.robert@ttk.hu

One of the most emerging scientific challenges today is the catalytic degradation of non-biodegradable polymers into value-added chemical feedstocks. The mild pyrolysis of polyolefins including high density polyethylene (HDPE) results in pyrolysis oils containing long-chain olefins as major products. Bicyclic alkyl amino carbene **(BICAAC)-Ru** temperature-induced latent olefin metathesis catalysts have been developed, which can be used for catalytic decomposition of long-chain olefins to propylene. These novel and thermally stable catalysts show significantly higher stability and activity at 75 °C comparing to 2nd generation Hoveyda-Grubbs (**HG2**) or cyclic alkyl amino carbene **(CAAC)-Ru** catalysts at ethenolysis condition. The conversion of long-chain olefins (e.g. 1-octadecene or methyl oleate) to propylene *via* isomerization metathesis (ISOMET) is performed by using $(RuHCl(CO)(PPh_3)_3$ (**RuH**) isomerization co-catalyst. The reactions can be carried out at as low as 1 ppm **BICAAC-Ru** catalysts loading at elevated reaction temperature (75 °C). The observed turnover number (TON) and turnover frequency (TOF) are as high as 55000 and 10000 $mol_{propylene} \cdot mol_{catalyst}^{-1} \cdot h^{-1}$, respectively. The bottleneck of the ISOMET reactions is presumably the rate of the isomerization step.

The synthesis of novel **BICAAC-Ru** olefin metathesis catalysts and their application in catalytic decomposition of long chain olefins *via* ISOMET using **RuH** isomerization co-catalyst will be presented.

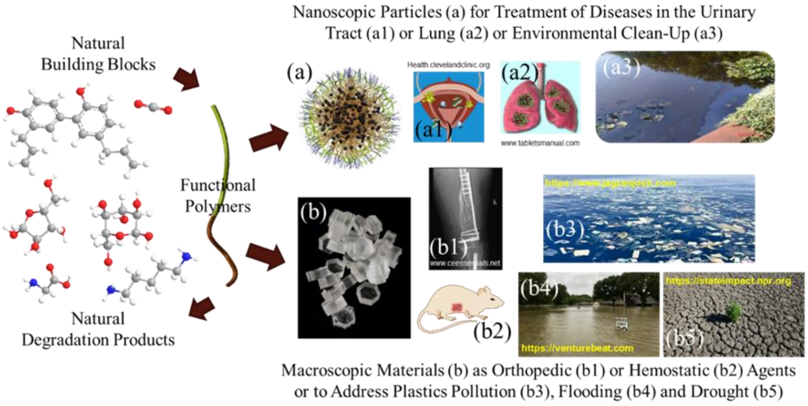
SYNTHETIC STRATEGIES BY WHICH TO AFFORD NATURAL PRODUCT-BASED POLYMER MATERIALS: IMPACTS ON SUSTAINABILITY, LIFE, HEALTH AND THE ENVIRONMENT & A FEW LESSONS FROM BOB

Karen L. Wooley

Departments of Chemistry, Chemical Engineering, and Materials Science & Engineering
Texas A&M University, College Station, Texas, USA
wooley@tamu.edu, @karen_wooley

A primary interest in the Wooley laboratory is the production of functional polymers from renewable sources that are capable of reverting to those natural products once their purpose has been served. A long-standing focus has been the development of synthetic methodologies that transform sugars, amino acids and other natural products into polymer materials. This approach allows for the production of functional polymers from renewable sources that are capable of reverting to those natural products once their purpose has been served (as is illustrated on the left side of the diagram below). This holistic life cycle approach is of importance from the perspectives of sustainable sourcing of materials feedstocks, while creating mechanisms for breakdown of the polymer materials after useful lifetime is complete, and providing for biological and environmental resorption of breakdown products. The overall process impacts the need to address the increasing accumulation and associated hazards of plastic pollution from the environmental persistence of non-degradable, petrochemically-sourced polymer systems. Moreover, inherent diversities of natural products provide opportunities to expand the scopes, complexities and properties of polymers, by utilizing fundamental organic chemistry approaches.

Target materials are designed for potential applications in diverse areas. For instance, we have produced amphiphilic block polymers that undergo supramolecular assembly in water to afford well-defined nanoscopic particles (diagram below, upper section (a)). By tuning the composition, structure and morphology, we are able to build functional nanoparticles that demonstrate efficacy as therapeutic nanomedicines for treatment of recurrent urinary tract infections (a1) and lung infections (a2). When the amphiphilic block polymers are co-assembled with iron oxide nanoparticles, magnetically-responsive organic-inorganic composite nanosystems result, which are able to perform as environmental remediation agents that capture >10x their mass in crude oil from contaminated water (work that began following the Deep Water Horizon oil spill more than a decade ago). Macroscopic forms (diagram, lower section (b)) of our Sugar Plastics™ were initially studied with an aim toward their use in orthopedic applications (b1), when we identified that specific chemical compositions containing nanoscopic and microscopic porosities operate as bioresorbable hemostatic wound dressing materials (b2). We're currently working with Teysha Technologies, LTD to advance these polymer materials for commercial translation as naturally-degradable plastic packaging to address the growing plastics pollution crisis (b3). In response to increasing challenges with climate change, we've designed analogs to exhibit properties that allow them to serve as superabsorbent degradable polymers to capture excessive liquid water, thereby preventing flooding, and later degrade to release the natural building blocks and water, thereby mediating drought and promoting crop growth (work that began from struggling through Hurricane Harvey in 2017). Most recently, we've turned our attention to the sourcing of the natural product feedstocks and are beginning to investigate strategies toward insect harvesting.



This presentation will highlight synthetic strategies for the development of polymers, block polymers and crosslinked network materials, which can be produced by relatively simple approaches from carbohydrates, amino acids and other natural small molecule or macromolecular components, and can be made to exhibit a range of properties. Target materials are designed for potential applications in diverse areas, from energy, *e.g.*, in electronic devices or batteries, to medicine, *e.g.*, as nanotherapeutics or bioresorbable hemostatic agents, to the environment, *e.g.*, as pollutant capture agents, climate resilient hydrogel materials or naturally-degradable plastics. Examples will highlight contributions that polymer chemistry can make toward bulk technological materials that are capable of impacting global needs, such as water-food-energy-health, and the grand challenges that must be solved in the coming decade, while also emphasizing fundamental synthetic chemistry advances.

Advanced Chemical Processes and Product Design for a Better World

^{1}H-^{15}N HMBC SPECTRA FOR ORGANIC MOLECULAR STRUCTURE DETERMINATIONS

Haw-Lih Su,[1] Rajeesha Rajan,[2] Yousef Mohammad Hijji,[2] Mohanad Ghazi Mohammed Shkoor[2]

[1]Central Laboratories Unit, Qatar University

[2]Department of Chemistry and Earth Sciences, Qatar University

hawlih@gmail.com

Nitrogen is one of the most common elements in organic chemistry. The various oxidation states and bonding choices of nitrogen generate disparate functional groups. The nitrogens are often the centers of chemical reactions, too. However, although nitrogen NMR spectroscopy has been known for long, it is rarely used in organic chemistry study. This is due to ^{14}N's and ^{15}N's low gyromagnetic ratios, ^{14}N's nuclear spin of 1, and ^{15}N's low nature abundance. Usually the measurements of nitrogen NMR spectra relay on ^{15}N isotope labelling or very long acquisition time, which are usually not affordable in organic chemistry study.

HMBC (Heteronuclear Multiple Bond Correlation) is a 2D NMR technique measuring the through-bond correlations inside a molecule. Recently we found ^{1}H-^{15}N HMBC experiment could efficiently address the issue of long acquisition time, providing promising information to verify the nitrogen-containing functionalities. In addition, the ^{1}H-^{15}N long range correlations provide very useful structure information. Here we will explain how ^{1}H-^{15}N HMBC technique could significantly reduce the measurement time and provide benefits on the structure determinations of organic molecules. Determining the product structures brought us better opportunities to obtain new reaction processes and controls.

AN ECO-FRIENDLY APPROACH FOR IMPROVED METHANE HYDRATE KINETICS IN NEAR-AMBIENT TEMPERATURE AND MODERATE PRESSURE

Ahmed Omran[1], Nikolai Nesterenko[2], Valentin Valtchev[1]

[1]Normandie Université, ENSICAEN, UNICAEN,CNRS, Laboratoire Catalyse et Spectrochimie (LCS), 14050, Caen, France
[2]TotalEnergies One Tech Belgium, Zone Industrielle C, 7181, Seneffe, Belgium
E-mail:omran@ensicaen.fr

Abstract:
The recent sanitary crisis and the following geopolitical disturbances have resulted in a severe unbalance between supply and demand and highlighted the need for economic and long-term natural gas storage. In that context, synthetic gas hydrates (**SGH**) or "*zeolitic ice*" arises as a promising technology to safely store methane in a sable, compact, and cost-efficient mode. However, SGH industrial application is mainly hindered by its slow formation kinetics as well as the cooling cost. To overcome those problems, research studies investigated using novel reactor designs and chemical additives as kinetic hydrate promoters (**KHPs**). However, the proposed reactor designs did not result in satisfactory results while common surfactant KHP such as SDS (sodium dodecyl sulfate) showed seriuos foaming problem especially when scaled-up [1,2] . In this study, we proposed an integrated approach of innovative reactor design and environmentally benign hydrate promoters. In this hybrid approach, the modified non-stirring tank reactor equipped with special corrosion-resistant packing has improved both mass and heat transfer without significantly affecting the overall storage capacity. In absence of any KHP, the new reactor configuration has reduced the induction time and **t_{90}** (time required to reach 90% of the final methane uptake) for mixed CH_4-THF hydrates at 6 MPa and 293.2K by 26% and 47%, respectively. Acidic zeolites and amino acids are two classes of novel green kinetic promoters that can enhance hydrate kinetics. The biodegradable amino acid (L-Tryptophan, L-Leucine) and eco-friendly acidic zeolite (H-SSZ-13) were studied with concentrations as low as 300 ppm to enhance mixed CH_4-THF hydrate kinetics at 6 MPa. The improved gas-liquid surface contact area has tremendously reduced the induction time, methane gas uptake, and t_{90} compared to blank THF and other studies reported in the literature. Acting as sites for heterogeneous nucleation, experimental observations showed that the presence of environmentally friendly hydrophobic promoter H-SSZ-13 outperformed the amino acids in the study. *The combined approach of reactor design and acidic zeolite promoter has reduced the induction time by 5 times and minimized the t_{90} by 64% while maintaining the methane gas conversion.* Finally, the performance of amino acids used has been accessed by DFT calculation and a direct relation between binding energy and promoter efficiency has been established. This simple approach can pave the way to control hydrate kinetics for developing and scaling up green and economical SNG processes.

Figure 1Illustration of integrated approach for enhanced methane hydrate formation kinetics.

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ASYMMETRIC SYNTHESIS OF 4,5-DIHYDRO-1H-[1,2,4]TRIAZOLE USING CARBOHYDRATES AS CHIRAL SCAFFOLDS

Anwaar S. Al Maqbali, Wajdi M. Zoghaib, John Husband, Raid J. Abdel-Jalil*

Chemistry Department, College of Science, Sultan Qaboos University, Muscat, Oman
E-mail: anwaaralmqbali94@gmail.com, Jalil@squ.edu.om

A novel series of enantiopure chiral 4,5-dihydro-1H-[1,2,4]-triazole appendage with acetylated mono-sugar moiety was synthesized by coupling hydrazonyl chlorides with the corresponding carbohydrate Schiff base derivatives in the presence of excess amount of triethyl amine *via* 1,3-dipolar cycloaddition reaction.

Methyl 2-arylhydrazono-2-chloroacetates were prepared via Japp-Klingmann reaction involving the coupling of arenediazonium salts to methyl 2-chloroacetoacetate. The synthesized compounds were characterized by ^{1}H & ^{13}C NMR, and FT-IR. The NMR results, especially the coupling constant values, prove the $^{4}C_{1}$ conformation of the products. Optical studies revealed that all the compounds reported here exhibited fluorescent emission of blue or green-yellow light and absorption at approximately 400 nm. Density functional theory (DFT) calculations will be used to explore the origin of the stereoselectivity observed in the 4,5-dihydro-1H-[1,2,4]-triazole reactions. Anti-tumour activity investigation will be performed on the synthesized compounds by National Institute of Cancer (NCI) in USA.

Keywords: *Heterocycles, Triazole, Enantiomers, Chiral heterocycle, Drugs, Carbohydrates, Glucopyronised, DFT, anti-tumour, sterioselectivity, asymmetric synthesis.*

BIOLOGY-ORIENTED DRUG SYNTHESIS OF GABAPENTIN DERIVATIVES: THEIR *α*-GLUCOSIDASE INHIBITORY ACTIVITY AND MOLECULAR DOCKING STUDIES

Sana wahid[1], Sajid Jahangir[1], Muhammad Ali Versiani[1], Khalid Mohammed Khan[2,3], Arshia[2]
[1]Department of Chemistry, Federal Urdu University of Art, Science, and Technology, Karachi, Pakistan
[2]H. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan
[3]Department of Clinical Pharmacy, Institute for Research and Medical Consultations (IRMC), Imam Abdulrahman Bin Faisal University, P.O. Box 31441, Dammam, Saudi Arabia
Email: Sanawahid90@gmail.com

Current research deals with the biology-oriented drug synthesis (BIODS) of twenty-one new thiourea analogs of pharmacologically important drug gabapentin, a well-known neuroleptic drug that is used as an anticonvulsant [1]. Structural characterization of all compounds was done by various spectroscopic techniques. Compounds **1–21** were subjected to *α*-glucosidase inhibitory activity *in vitro*. Screening results revealed that the whole library was found to be active having IC_{50} ranges from 0.40 ± 0.14 *μ*M to 37.60 ± 1.33 *μ*M. It is noteworthy that several derivatives including **26** (IC_{50} = 2.69 ± 1.53 *μ*M), **28** (IC_{50} = 0.83 ± 0.60 *μ*M), **29** (IC_{50} = 1.58 ± 0.73 *μ*M), **30** (IC_{50} = 0.82 ± 0.15 *μ*M), **32** (IC_{50} = 1.90 ± 0.69 *μ*M), **33** (IC_{50} = 0.40 ± 0.14 *μ*M), **34** (IC_{50} = 1.30 ± 0.18 *μ*M), **37** (IC_{50} = 0.74 ± 0.22 *μ*M), **40** (IC_{50} = 0.82 ± 0.17 *μ*M), **43** (IC_{50} = 1.04 ± 0.28 *μ*M), and **44** (IC_{50} = 0.88 ± 0.38 *μ*M) showed *α*-glucosidase inhibition greater than standard acarbose (IC_{50} = 2.05 ± 0.41 *μ*M). While compounds **24** (IC_{50} = 2.69 ± 1.53 *μ*M), **35** (IC_{50} = 3.02 ± 0.44 *μ*M), **38** (IC_{50} = 2.07 ± 1.7 µM), 39 (IC 50 = 1.57 ± 0.91 µM) showed greater α-glucosidase inhibition than gabapentin (IC_{50} = 3.91 ± 0.65 *μ*M). A most probable structure-activity relationship (SAR) was anticipated by observing the varying degree of inhibitory potential given by compounds. However, molecular insights regarding the binding mode of gabapentin thiourea analogs within the active pocket of *α*-glucosidase were rationalized by molecular docking studies.

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CO-AGGREGATION OF S100A9 WITH L- DOPA AND CYCLEN-BASED COMPOUNDS SHOWED AMYLOID FIBRIL THICKNING WITHOUT ALTERING RATES OF SELF-ASSEMBLY

L. Arabuli[1,2], I. A. Iashchishyn[1], N. V. Romanova[1], G. Musteikyte[3,] V. Smirnovas[3], H. Chaudhary[1], Ž. M. Svedruži´c[4], and L. A. Morozova-Roche[1]

[1]Department of Medical Biochemistry and Biophysics, Umeå University, SE-90781 Umeå, Sweden
[2]Department of Natural Sciences, School of Science and Technology, University of Georgia, 0171 Tbilisi, Georgia
[3]Institute of Biotechnology, Life Sciences Center, Vilnius University, LT-10257 Vilnius, Lithuania
[4]Department of Biotechnology, University of Rijeka, HR-51000 Rijeka, Croatia
E-mail: l.arabuli@ug.edu.ge

We consider the effect of cyclic compounds and their conjugates on the amyloid formation of pro-inflammatory S100A9 protein, which was found to be a common denominator in Alzheimer’s and Parkinson’s disease as well as in traumatic brain injury, which is considered as a pre-cursor state for neurodegenerative ailments [11,12]. Indeed, amyloid formation is commonly associated with neuroinflammation, and pro-inflammatory S100A9 protein acts both as an alarmin, inducing the production of pro-inflammatory cytokines, and as a highly amyloidogenic protein, which self-assembles into amyloids under physiological conditions.

The amyloid cascade is central for the neurodegeneration disease pathology, including Alzheimer’s and Parkinson’s, and remains the focus of much current research. S100A9 protein drives the amyloid-neuroinflammatory cascade in these diseases. DOPA and cyclen-based compounds were used as amyloid modifiers and inhibitors previously, and DOPA is also used as a precursor of dopamine in Parkinson’s treatment. Here, by using fluorescence titration experiments we showed that five selected ligands: DOPA-D-H-DOPA, DOPA-H-H-DOPA, DOPA-D-H, DOPA-cyclen, and H-E-cyclen, bind to S100A9 with apparent Kd in the sub-micromolar range. Ligand docking and molecular dynamic simulation showed that all compounds bind to S100A9 in more than one binding site and with different ligand mobility and H-bonds involved in each site, which all together is consistent with the apparent binding determined in fluorescence experiments. By using amyloid kinetic analysis, monitored by thioflavin-T fluorescence, and AFM imaging, we found that S100A9 co-aggregation with these compounds does not hinder amyloid formation but leads to morphological changes in the amyloid fibrils, manifested in fibril thickening. Thicker fibrils were not observed upon fibrillation of S100A9 alone and may influence the amyloid tissue propagation and modulate S100A9 amyloid assembly as part of the amyloid-neuroinflammatory cascade in neurodegenerative diseases.

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COPPER(II) THIOSEMICARBAZONE COMPLEXES OF BIOLOGICAL RELEVANCE

IMAN AL SALMI,[1] **MUSA SHONGWE**,[1] **CRAIG ROBERTSON**
[1] *Department of Chemistry, College of Science, Sultan Qaboos University, Sultanate of Oman*
[2]*Department of Chemistry, University of Sheffield, UK*
E-mail: s7720@student.squ.edu.om

There is considerable current interest in thiosemicarbazones ligands due in part to their structural diversity, multidonor properties and their tendency to exhibit biological activity, which is enhanced on coordination to bioactive transition metal ions. Thiosemicarbazones are well-known for their coordination versatility which derives largely from their propensity to undergo tautomerization as demanded by the central metal ion. They can be designed in various denticities for a wide range of purposes and synthesized straightforwardly. Such hydrazones, along with their corresponding transition-metal complexes, have inherent pharmacological properties and display fascinating physicochemical features.[1]

Some copper and iron complexes with α-*N*-heterocyclic carbaldehyde thiosemicarbazones have been demonstrated to model the active site of ribonucleotide reductase, a key enzyme in the synthesis of precursors of DNA.[2] Over the years, copper(II) complexes with thiosemicarbazones have featured prominently in DNA-cleavage studies. Moreover, such complexes have been investigated for cytotoxicity against cancer cell lines and shown to exhibit antiproliferative activity. They also display antimicrobial properties.[3]

In this work, we have designed, synthesized and isolated a diverse range of novel ternary complexes of copper(II) comprising thiosemicarbazones and phenanthroline derivatives. The 3-D structures have been determined by single-crystal X-ray analyses which revealed the effect of the tetragonal distortion. By virtue of being paramagnetic, these compounds have been characterised by magnetic susceptibility measurements and electron spin resonance spectroscopy. They show remarkable antibacterial and anticancer activities.

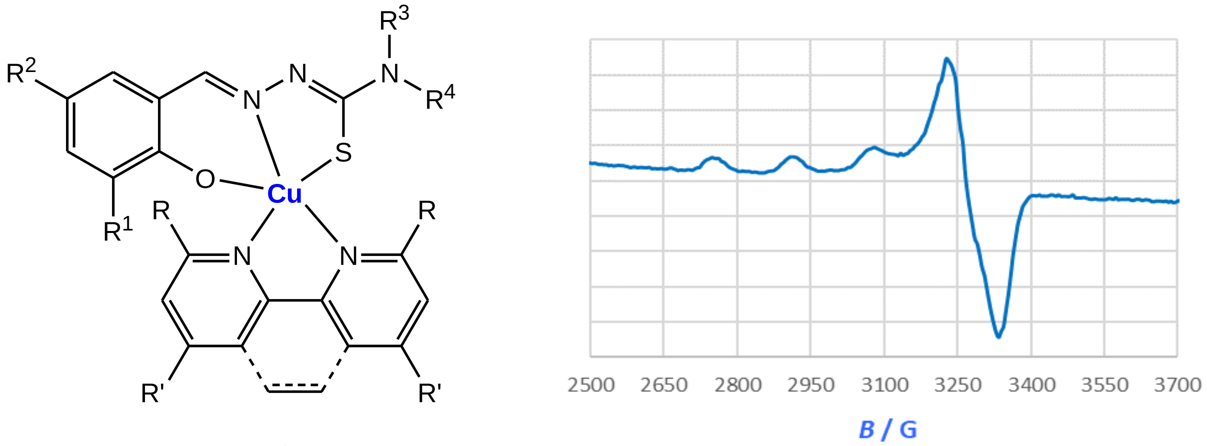

Figure 1: General structure of a ternary copper(II) thiosemicarbazone complex and a typical X-band ESR at LN temperature

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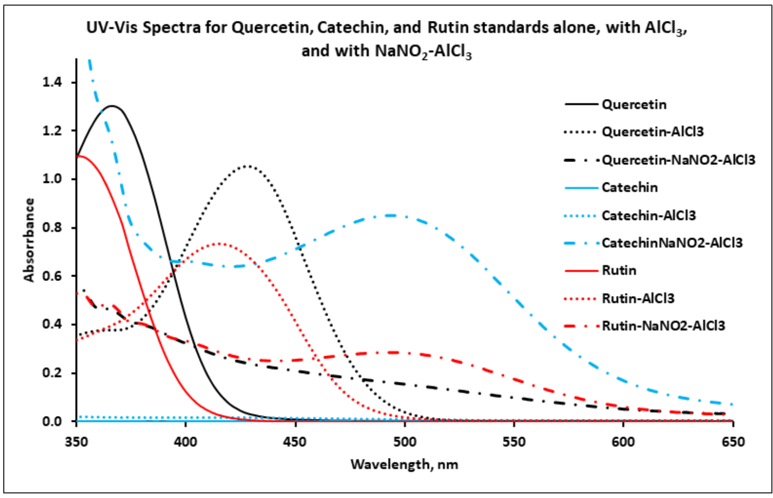
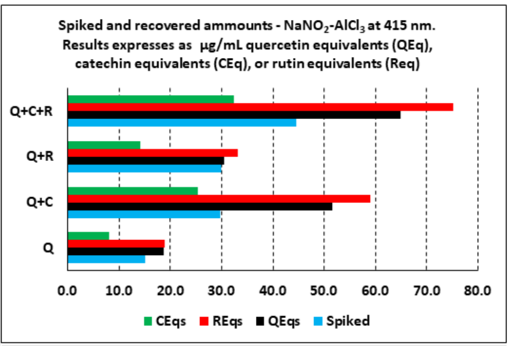
CRITICAL EVALUATION OF THE ALUMINIUM CHLORIDE ASSAY FOR THE DETERMINATION OF TOTAL FLAVONOID CONTENT

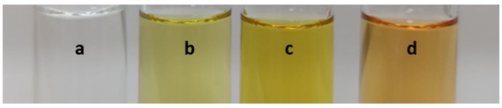
Amjad M. Shraim [1], **Talaat A. Ahmed** [2], **Md Mizanur Rahman** [3], **Yousef M. Hijji** [1]

[1] *Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University, PO Box 2713, Doha, Qatar*
[2] *Environmental Science Center, Qatar University, PO Box 2713 Doha, Qatar*
[3] *Department of Biological and Environmental Sciences, College of Arts and Sciences, Qatar University, PO Box 2713, Doha, Qatar*
Email: amjad@qu.edu.qa

The aluminium chloride colorimetric ($AlCl_3$) assay is widely employed for the determination of total flavonoid content (TFC) in plant extracts. The assay quantifies TFC against authentic flavonoid standard assuming equal responses from all flavonoids available in the sample. The accuracy of the assay was assessed using spike recovery in plant extracts and authentic flavonoid standards. Due to huge differences in absorbance between flavonoids, the assay produced unacceptable differences in TFC when results are expressed as quercetin, rutin, or catechin equivalents. Employing the assay in standard solutions produced high false results when quercetin content was expressed as rutin equivalents or when rutin was expressed as quercetin equivalents. Similarly, unacceptable spike recoveries were obtained when using the assay in standard solutions. For plant extracts, unacceptable differences (58–152%) in TFC were also obtained when either quercetin or rutin was used as a standard. Likewise, unacceptable high or low recoveries were recorded when the assay is used in conjunction with sodium nitrate. Conclusive evidence about the dependency of the TFC on the flavonoid standard used for quantitation will be presented and discussed, which in turn highlight the inherent critical flaws of the assay.






(a) Reagent blank, (b) Sample, (c) Sample+$AlCl_3$, (d) Sample+$AlCl_3$+$NaNO_2$

ELECTROCHEMICAL TREATMENT OF GTL PROCESS WATER

Shaima A. Al-Tamreh , Muftah H. El-Naas*

[a] *Gas Processing Centre, College of Engineering, Qatar University, Doha, Qatar*

*Corresponding author: e-mail muftah@qu.edu.qa

The generation of considerable amounts of wastewater from the gas-to-liquid (GTL) process is a major concern in the gas industry. Severe environmental issues, such as water pollution, can be caused by the impacts of discharging untreated GTL wastewater. This wastewater is characterized by its high chemical oxygen demand (COD) which is resulting form several pollutants such as fatty acids, alcohols, aldehydes, and ketones. It also contains a high acidity that affects aquatic life. Thus, to meet the acceptable limit for discharging wastewater, several treatment methods can be utilized to reduce the amount of COD. Electrocoagulation (EC) technique can play a significant role in decreasing the COD value of GTL wastewater. The simplicity of EC offers a substantial advantage in treating this type of wastewater. A direct-current power supply and at least two conductive electrodes are required for producing in-situ coagulants. Using these coagulants gives more economic advantages than chemical coagulants (which require the addition of expensive chemicals). In this work, a patent electrode was examined to enhance the EC efficiency of GTL process water treatment. A perforated cathode was designed to reduce the passivation by providing aeration through holes. Various ranges of pH, current densities, and conductivities were studied to evaluate the efficiency of EC in reducing COD content in the GTL process water. EC showed high performance in treating GTL to reduce COD and other undesired pollutents. Detailed experimental results and process optimization will be presented.

Metabolic Ketoacidosis Detection- An In Vivo Approach

Mizaj Shabil Sha[1], Muni Raj Maurya [1,2], Sadiyah Shafath[1,3], John-John Cabibihan[2], Abdulaziz Al-Ali[4,5], Rayaz A. Malik[6] and Kishor Kumar Sadasivuni[1,] *

[1]Center for Advanced Materials, Qatar University, PO Box 2713, Doha, Qatar.

[2]Department of Mechanical and Industrial Engineering, Qatar University, PO Box 2713, Doha, Qatar.

[3] Department of Chemical Engineering, Qatar University, PO Box 2713, Doha, Qatar.

[4]Department of Computer Science and Engineering, Qatar University, PO Box 2713, Doha, Qatar

[5]KINDI Center for Computing Research, Qatar University, Doha, Qatar

[6]Weill Cornell Medicine-Qatar, Qatar Foundation-Education City, PO Box 24144, Doha, Qatar

*Corresponding author: kishor_kumars@yahoo.com

Abstract

Detecting euglycemic ketoacidosis in individuals with type 1 or type 2 diabetes or heart failure treated with SGLT2-i is crucial which ultimately results in glycemia, renal function, cardiovascular outcomes and all-cause mortality. For the rapid and noninvasive detection of ketoacidosis, a colorimetric visual sensor for measuring breath biomarker was designed. Using dye solutions as sensing elements, a portable and low-cost IoT-based prototype with full functionalities for detecting breath biomarkers within 60 seconds was developed. The response time, pH effect, temperature impact, and concentration effect of a highly specific multiple-dye system was used to estimate breath acetone levels. In the detection range of 0.05-50 ppm, we established a detection limit of 0.0217 ppm for acetone and 0.029 ppm for ethanol using the proposed method. The effective applications of this unique technique as a visual sensor platform in the biological area and the domain of environmental chemistry have significant potential.

METAL-ORGANIC FRAMEWORKS FOR THE PHOTONIC FIXATION OF NITROGEN TO AMMONIA: A COMPUTATIONAL AND EXPERIMENTAL STUDY

Amro M. O. Mohamed,[1] Alessandro Sinopoli,[2] Yusuf Bicer,[1]
[1]Division of Sustainable Development, College of Science and Engineering, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar
[2]Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Qatar Foundation, Qatar
E-mail: ammohamed@hbku.edu.qa

Photofixation of nitrogen is one of the most important phenomena that govern the completion of the nitrogen cycle. To diverge into synthesizing ammonia with a less intensive and less pollutant process, photoactive material that assimilated light energy is triggered to generate electrons. Numerous studies have been conducted to bring photofixation into the practical side of ammonia production. Distinct material compositions have been investigated starting from the mid-70s; however, until now, photocatalysts suffer from low ammonia yield and incomprehensive understanding of the mechanism. Catalysts provide an alternative path by lowering the activation energy requirement, speeding up the chemical reaction. This research aims to develop a systematic and comprehensive approach to designing durable and efficient catalysts that can drive the photofixation of nitrogen. By utilizing Quantum mechanics, molecular simulations techniques, structural and mechanical properties, libraries of metal-organic frameworks (MOFs) are screened to identify a set of promising catalysts for the photofixation of nitrogen. Beside technical assessment, the methodology considers all sustainability aspects; energy, environment, and logistics sides. Life cycle thinking is implemented in this work, and selected impact assessment categories quantify the overall environmental load of a particular set of catalytic materials. Consequently, selected materials are synthesized characterized, and their performance is evaluated for the process in a photoreactor. The work emphasizes the importance of bridging the gap between the design of ideal catalysts and actual performance.

We primarily used density functional theory (DFT) and molecular simulation (Monte Carlo and Molecular Dynamics) techniques to identify MOFs with appropriate electronic and structural properties. The top candidates have been examined from the perspective of guest molecules' adsorption and diffusion MOFs' geometrical, mechanical, and chemical stability properties. As a result of a study on Hypothetical MOFs, $Zn_3(BTC)_2(C_6H_5)$ has been shown to satisfy the requirement for photofixation of nitrogen, using hydrogen and nitrogen as raw materials ammonia. On a different screening based on an experimental-based dataset, most potential materials from the screening were Fe-based MOFs using water as the source of hydrogen. Four MOFs, Fe_2Cl_2(BBTA), Fe_2(mDOBDC), Zn_2(mDOBDC), and Ni-BTP, have been selected based on their band edges, while only Fe_2Cl_2(BBTA) MOF exhibited a bandgap less than 3 eV. Among the four MOFs, Fe_2(mDOBDC) exhibited the highest shear modulus of approximately 31 GPa. Moreover, we propose 48 MOFs' combinations for heterojunction application to enhance charge carriers' separation. Intriguingly, we demonstrated the predictability of MOF's bandgap and edges from MOF's organic linker bandgap and metal node type (oxidation state and corresponding electronic configuration) for some MOFs' families. Environmental impact of producing a gram of Fe_2Cl_2(BBTA), Zn_2(mDOBDC), Fe_2(mDOBDC), and Ni-BTP results in 2.19, 1.49, 1.33, and 0.35 kg CO_2 (eq.) of total global warming potential emissions.

A selected number of MOFs are synthesized using the solvothermal method and characterized using various techniques. These MOFs were tested for activity towards nitrogen fixation under visible-light irradiation. This work also explores the feasibility of the solar-based nitrogen fixation process from an economic perspective and compares it with the traditional process. One of this research's main objectives is to set a performance target for efficiency, production rates, and scale to achieve economic feasibility. If considering five years of break-even point, the current ammonia yield must be increased to nine-folds of the current experimental laboratory conversion.

Midwakh: What Do We Know Today? Chemical and Health Assessment of Dokha

Yehya El Sayed*, Fatin Samara, Maissam El-Kouche, and Isra Alam

Department of Biology, Chemistry and Environmental Sciences, American University of Sharjah

*Corresponding author email: yehyaelsayed@gmal.com

Tobacco use is one of the leading preventable causes of death around the world. There has been a decline in cigarette smoking over the last ten years; however, this has been accompanied by an increase in the popularity of alternative tobacco products (ATPs), which has become a public concern. While most recent research has concentrated on e-cigarettes and waterpipes (hookah), little is known about another ATPs product known as dokha, which is smoked through a pipe called medwakh. Dokha is a type of alternative tobacco product (ATP) made from tobacco leaves and additives in a specific process. Dokha, a traditional tobacco grown in the Arabian Gulf region, has become increasingly popular among high school students and adults in the region. Dokha is trending in countries other than the Arabian Gulf region, according to web searches, including Russia, the United Kingdom, and the United States. This increased interest suggests that dokha is gaining popularity and may become an epidemic in the future, similar to waterpipes. In this research, the dokha smoking topography was generated. The smoke was then produced using a device that mimicked human puffing, and the smoke was then trapped on adsorbent tubes. The chemical compositions of raw dokha samples and smoke were determined using gas chromatography mass spectrometry, thermal analysis, and elemental analysis. The analysis revealed the presence of several potentially harmful compounds in dokha smoke, including irritants, carcinogens, and CNS depressants. Dokha smoke contained over 400 chemical compounds. Toxic metals were found in dokha samples in concentrations comparable to, if not greater than, those found in cigarettes. Also, nicotine and polycyclic aromatic hydrocarbons (PAHs) concentrations in raw and smoked dokha samples were determined. The nicotine content of raw dokha far exceeded that of cigarettes, cigars, waterpipes, and chewing tobacco. Despite the fact that only a portion of the nicotine is released into the smoke, the amount of nicotine in dokha smoke was higher than that reported for cigarettes. The toxic equivalency quotient, daily exposures, incremental lifetime cancer risk, and hazard quotient were all calculated using PAH concentrations. Two PAHs were found in trace amounts in raw dokha, and 12 PAHs were found in dokha smoke in amounts that exceeded those found in cigarette smoke. The distribution of PAHs in smoke revealed a distinct pattern and a higher risk factor than that found in cigarettes and other tobacco products.

MINERAL CARBONATION OF STEEL-MAKING WASTE IN REJECT BRINE: OPTIMIZATION APPROACH

Mohamed H Ibrahim[1], Nafis Mahmud[1], Muftah H. El-Naaas[1*]

[1]*Gas Processing Center, Qatar University, P.O. Box 2713, Doha, Qatar*

E-mail: muftah@qu.edu.qa

Carbon capture and sequestration (CCS) is a major player in mitigating climate change. CCS includes a portfolio of technologies that can possibly capture vast amounts of CO_2 per year. Mineral carbonation (MC) is a possible candidate to sequester CO2 from medium-sized emissions point sources. The active alkaline elements are the fundamental reactants for MC. Industrial wastes emerge as an alternative source of carbonation minerals that have higher reactivity than natural minerals; they are also inexpensive and readily available in proximity to CO_2 emitters. Steel-making wastes exhibit alkaline properties since it contains calcium and magnesium oxides. In this work, accelerated carbonation of steel-making dust in reject brine has been evaluated in an Inert Particles Spouted Bed Reactor (IPSBR) which is specially designed for contacting three-phase mixtures. A factorial experimental design was used to classify the effects of the operating parameters (solid to liquid ration, CO_2 gas flowrate and inert particles fraction) on the CO_2 uptake in semi-batch mode. The analysis of the experimental results indicated that the optimum CO_2 uptake was 0.22 g CO_2/g waste. The best CO_2 uptake performance (0.977 gCO2/g waste) was achieved at ambient temperature and pressure of 5 bar. The optimum conditions were then used to run the experiment in continuous mode which resulted in 96% CO_2 removal.

MOLECUAR SIMULATION: A POWERFUL DESIGN TOOL FOR FISCHER-TROPSCH SYNTHESIS

Ioannis G. Economou,[1] **Konstantinos D. Papavasileiou,[2] Loukas D. Peristeras[2]**

[1]*Texas A&M University at Qatar, Chemical Engineering Program, Education City, PO Box 23874, Doha, Qatar*
Corresponding author e-mail: ioannis.economou@qatar.tamu.edu
[2]*National Center for Scientific Research "Demokritos", Institute of Nanoscience and Nanotechnology, Molecular Thermodynamics and Modelling of Materials Laboratory, GR-15310 Aghia Paraskevi Attikis, Greece*

The Fischer-Tropsch (FT) route is a polymerization reaction used extensively in the Gas-to-Liquids (GTL) process to transform natural gas [1] into high quality, low emission transportation fuels. The main FT reaction products, namely water, wax and small amounts of oxygenates, form a mixture through which the dissolved reactants diffuse, reach the catalytic nanoparticles and react. The industry has been long interested in the fundamental aspects of FT reactor modelling with high fidelity to provide guidance in GTL process optimization. Reactant diffusivities and solubilities in GTL wax are two pivotal aspects to achieve a reliable reactor model. To this end, we developed an accurate predictive model for these properties using Molecular Dynamics (MD) simulations with state-of-the art atomistic force fields for H_2, CO and H_2O in the wax at temperatures and pressures corresponding to the actual GTL industrial conditions [2-4]. Recently, MD simulations were performed to evaluate the performance of several force fields on the reproduction and prediction of liquid densities, surface tension and viscosities over a broad temperature range for n-C_{12}, n-C_{28}, their binary mixture, and a model mixture of the commercially available SX-70 wax [5]. The experimental validation highlighted the strength of MD simulations as a valuable and reliable tool for basic physical property predictions.

Additional work focused on simulations of prototype GTL mixtures under confinement in order to resemble their behavior inside the catalyst pores. FT catalysts deactivate over time and excess water conditions can cause sintering of catalytic nanoparticles (NP). Using atomistic (AA) and coarse-grained (CG) simulations, we studied n-C_{28} – water mixtures inside TiO_2, pristine graphene and graphene oxide mesopores with emphasis on excess water conditions [6-7]. Both methods captured the mixture phase separation and the component diffusivity as a function of the distance from the pore center, predictions confirmed by phase behavior NMR in porous silica [8]. Grand Canonical Monte Carlo (GCMD) simulations also showed that the Co NP does not affect the mixture phase separation; however, it is extensively covered by water. Given the experimental difficulties in probing the relevant mechanisms at this scale, our results expected to open new pathways in the investigation of the effect of NPs on catalyst support interfaces in the presence of FTS mixtures.

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MOLECULAR SIMULATION OF 6FDA-DAM MIXED MATRIX MEMBRANES FOR CO_2/CH_4 SEPARATION

Marcelle B M Spera[1], **Panagiotis Krokidas**[2], **Ioannis G. Economou**[1]

[1]*Chemical Engineering Program, Texas A&M University at Qatar, Education City, Doha PO Box 23874, Qatar*
[2]*National Center for Scientific Research "Demokritos", Institute of Nanoscience and Nanotechnology, Molecular Thermodynamics and Modelling of Materials Laboratory, 15310 Aghia Paraskevi Attikis, Greece*
E-mail: marcelle.spera@qatar.tamu.edu

Significant progress has been made on the fabrication of metal-organic framework (MOF) membranes over the last decade [1]. Nevertheless, scalability and cost are still a great challenge for industrial application of these membranes. A promising alternative that has been described [2] as an evolutionary approach towards the advancement from polymeric membranes to inorganic high-performance membranes is the so-called mixed matrix membrane (MMM). This composite membrane uses a polymer as support for MOF particles, which are referred to as fillers. With inorganic particles dispersed in the membrane, one can take advantage of the polymer scalability, low cost, and excellent mechanical strength and improve its separation performance by adding particles with well-defined pore sizes that could be tailored to the desired separation.

Due to the heterogeneity of the membrane, permeability prediction is not straightforward. Several theoretical models have been proposed to calculate gas permeability of MMM using parameters such as the permeability of the pure polymer, permeability of the MOF, and the volume fraction of the filler [3]. Nevertheless, to overcome the limitations of the models and the requirement of empirical adjustments, we can take advantage of molecular simulations to predict the performance of the membrane for a desired separation in a faster and cheaper way and guide experimental design and synthesis of the membrane material.

CO_2 separation is key to clean energy technologies. CO_2 capture from natural gas (CH_4) increases its energy density and also prevents pipeline corrosion during transport [4]. 6FDA-based MMM were reported to show good performance for CO_2/CH_4 separation [5,6]. Using non-equilibrium molecular simulations and theoretical models, we report in this work excellent predictions for the use of 6FDA-DAM MMMs for CO_2/CH_4 separation, all inside the so-called comercially-attractive region. Our MOFs are zeolitic-imidazolate frameworks (ZIFs) *in silico* designed by metal and linker substitution [7], with outstanding performance.

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NANO CARBON DOTS DERIVED FROM FISH WASTE AND ITS APPLICATION TO PROTECT THE MARINE MATERIALS

P Muhamed Ashraf*, VS Anju, PK Binsi

ICAR Central Institute of Fisheries Technology

Cochin 682 029.

Email: ashrafp2008@gmail.com

Abstract

Prawn, shrimp and crab shell discards from fish processing industries and domestic vending units impose serious environmental issues. To some extent, shrimp peeling waste is utilized for the extraction of chitin, caroteno-proteins and other organics. However, the conventional procedures to extract these materials involve environmentally benign acids and alkalies and also during these individual centric extraction processes, other economically important biomolecules such as pigments will be denatured or disintegrated. The present study aimed at simultaneous synthesis of carbon dots from prawn shell by utilizing its proteinaceous materials, chitin and calcium carbonate through a hydrothermal method. Further, the prepared carbon dots were used to reinforce Bisphenol A epoxy polymer and the corrosion inhibition efficiency of the reinforced polymer in boat building steel was assessed. Nano carbo dots synthesized from prawn shell was subjected to FTIR, UV-Vis spectrophotometry, fluorescence, SEM and atomic force microscopic studies. The electrochemical impedance spectral studies of the reinforced polymer exhibited highest polarization resistance and lowest capacitance when coated on boat building steel. CD reinforced epoxy polymer exhibited crack and pore free surface morphologies compared to that of control. The quality of chitin and calcium carbonate extracted after carbon dot separation was found to be superior to that extracted by conventional protocols as evidenced by FTIR and XRD studies. The hydrothermal extraction protocol standardized in the present study for the isolation of nano carbon dot, chitin, and calcium carbonate from prawn shell highlights a green, cheaper and environment friendly protocol for the synthesis of high value products from prawn shell discards.

OPTIMIZATION OF IONS REMOVAL AND CO_2 UPTAKE OF DESALINATION REJECT BRINE AS A PART OF AN INTEGRATED PROCESS FOR BRINE MANAGEMENT AND CO_2 SEQUESTRATION

Nafis Mahmud[1], Mohamed H Ibrahim[1], Daniela V. Fraga Alvarez[2], Ahmed Khodary[3], Daniel V. Esposito[2], Muftah H El-Naas[1*]

[1]*Gas Processing Center, Qatar University, P.O. Box 2713, Doha, Qatar*

[2]*Department of Chemical Engineering, Columbia University in the City of New York, 500 W. 120th St., New York, NY 10027, United States of America*

[3]*Qatar Shell Research and Technology Center, Doha, Qatar*

*E-mail:muftah@qu.edu.qa

A multistage process scheme for extracting valuable minerals from desalination reject brine while simultaneously sequestering CO_2 has been proposed. First part of the the proposed scheme involves the removal of magnesium ions via addition of NaOH. The magnesium-free brine effluent was then reacted with CO_2 in presence of NaOH for simultaneous removal of calcium ions and CO_2 sequestration in an inert particle spouted bed reactor (IPSBR). Response surface methodology was applied to optimize the effect of various process parameters on both stages of the proposed scheme with the target of maximizing magnesium removal in the first stage, and maximizing calcium removal and CO_2 uptake in the second. A second-order regression model was generated for each individual target response. The predicted responses for all targets were in good agreement with the obtained experimental values. The optimum conditions for the process parameters for the two stages were also determined. Results indicated that 98.8% of magnesium can be removed in the first stage at brine salinity, NaOH dose, and temperature of 73.5 g/L, 8.22 g/L and 45.5 °C, respectively. On the other hand, a multivariate optimization approach was adopted in the second stage based on which the optimum conditions for NaOH, flowrate and salinity for simultaneous calcium removal and CO_2 sequestration were found to be 5 g/L, 2 L/min and 75 g/L, respectively. Under these conditions, 100% removal of Ca^{2+} ions from the brine could be achieved with a CO_2 uptake of 5.4 g/L. Moreover, the solid products obtained under the optimum conditions were characterized confirming the formation of high purity magnesium hydroxides and calcium carbonates. The scheme can be further improved by incorporating an electrolysis unit to produce HCl along with NaOH that can be recirculated to eliminate the need for any external addition of NaOH thus creating a sustainable process for reject brine management and CO_2 sequestration.

PRODUCTION OF SUSTAINABLE AND ENVIRONMENTAL FRIENDLY BIODIESEL FROM CHICKEN FAT OIL USING HETEROGENEOUS CATALYST

Ammad Nasir[1], Fahad Javed[2], Fahad Rehman[2], Soban Qamar[1], Syed Nasir Shah[3]

[1]*Department of Mechanical Engineering, Faculty of Mechanical and Aeronautical Engineering, University of Engineering and Technology Taxila, Taxila 47080 Rawalpindi, Pakistan*

[2]*Microfluidics Research Group, Department of Chemical Engineering, COMSATS University Islamabad, Lahore Campus, Pakistan*

[3]*Department of Energy Engineering, Faculty of Mechanical and Aeronautical Engineering, University of Engineering and Technology Taxila, Taxila 47080 Rawalpindi, Pakistan*

Email: nasir.shah@uettaxila.edu.pk, nasir876@gmail.com

Biodiesel is nontoxic, biodegradable and environmentally friendly fuel which is most famous fuel in the eyes of researchers due to the absence of CO, CO_2, SOx and NOx and which can’t take part in green-house gas. Moreover, Biodiesel produced from chicken fat is considered as renewable form of energy as the meet requirement is increasing day by day. Moreover, the demand of chicken fat is also increasing due to increase in population each passing day. Hence, associated chicken fat waste is also increasing. Biodiesel is mostly produced through transesterification or simply esterification reaction process and it can be used as fuel for diesel engines, by mixing it with diesel or simple using 100% pure BD.

In this study, a clean, biodegradable and environmentally friendly biodiesel was produced from chicken fat oil to meet the global energy requirements and replace the usage of petroleum-based diesel which deteriorates the environment. Chicken waste is one of the largest wastes in Pakistan and may contain veterinary drugs, environmental pollutants, and natural contaminants that can harm human life as well as environment. On the other hand, chicken fat oil can be a low cost and readily available feedstock for biodiesel production that is sustainable and environmentally friendly form of energy. Sonication and microbubble technique were used in this study which are non-conventional methods that are used to get higher yield of biodiesel (95% and 96%) in relatively shorter period of reaction time (30 min).

KEYWORDS: Environmentally Friendly Biodiesel (BD), Sustainable Energy, Chicken Fat Oil (CFO), Microbubble, Sonication

SUPPORTED LIPID MEMBRANE INTERFACES FOR CELLULAR SIGNALING STUDIES

Kabir H Biswas[1]

[1]*College of Health & Life Sciences, Hamad Bin Khalifa University, Doha, Qatar*
Email: kbiswas@hbku.edu.qa

Cell membrane mimetic, synthetic supported lipid bilayers (SLBs) assembled on solid supports serve as an advanced, two-dimensional functional materials platform for a variety of applications including *in vitro* reconstitution of cellular signaling reactions [1-4]. Such applications of SLBs are largely enabled by the preservation of the lateral mobility of the lipid molecules, and any lipid-anchored biomolecule such as protein or deoxyribonucleic acid (DNA) molecules, allowing assembly of chemically-driven, natural-like receptor-ligand clusters leading to induction of cellular effects [3-7]. Additionally, application of nanolithography and micropatterning techniques to the SLB platform has provided a spatial control over the assembly of receptor-ligand clusters leading to the dissection of the role of spatial organization of receptor-ligand clusters in the cellular activities [1-2, 4-5]. In this talk, I shall describe the role of interfacial forces in the adhesion and spontaneous fusion of lipid vesicles during SLB assembly [8], and utilization of the SLB platform interfaced with living cells in a hybrid format in understanding the mechanism of cellular adhesion and mechanical force-mediated signaling [9-12]. Insights gained from these studies may provide therapeutic avenues targeting metastasis of cancer cells such as in the case of breast cancer, and generally project functionalized membrane surfaces as precision biointerfacial materials for future biomedical applications.

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TOWARDS A LOW CARBON CONCRETE: DEVELOPMENT OF CALCIUM SULFOALUMINATE-BASED CEMENT IN QATAR

Omnya Abdalla[1], Roneta Chaliulina[1], Marcus Nigel Campbell [2], Jose-Luis Galvez-Martos[3], Ammar Elhoweris [1, *]

[1]*Gulf Organization for Research and Development, Qatar Science and Technology Park, Doha, Qatar*

[2]*School of Engineering, University of Aberdeen, AB24 3UE, United Kingdom*

[3]*Systems Analysis Unit, IMDEA Energy, Avda. Ramón de la Sagra 3, Móstoles, Madrid E-28935, Spain*

[*] *Email: a.elhoweris@gord.qa*

Global climate change is primarily caused by greenhouse emissions. The cement industry contributes to about 5% of these emissions, as every ton of Ordinary Portland Cement (OPC) emits about 0.97 tons of CO_2, roughly half of which arises from the raw material decarbonation (calcination of limestone) and a half from the fuel required to reach reaction temperatures. Lowering the anthropogenic carbon emissions associated with cement industry could make a huge difference in our environmental impact, thus there is an urgent need to develop alternative cement formulations. Calcium sulfoaluminate (CSA) cements are promising candidates that can substitute OPC because of their rapid strength gain, shorter curing time, and lower shrinkage. Moreover, they possess eco-friendly characteristics related to low carbon emissions, as a lower quantity of limestone is used for production, thus calcination emissions are reduced. Nevertheless, the process still lacks economic viability due to the high cost of alumina, which is a key component in the ye'elimite phase of CSA cement and is responsible for the early-stage strength. One possible way to overcome the high cost is to use high-alumina clays, with lower alumina contents than bauxite to avoid competition with the aluminum industry. Another method is to reduce the ye'elimite content but, to compensate for the loss of strength, the reactive alpha-prime polymorph of dicalcium silicate could be introduced. In a novel technology developed by GORD, elemental sulfur is utilized as both fuel and a source of clinker sulfur oxide to synthesize alpha-prime dicalcium silicate and ye'elimite CSA cement. Several clinker formulations were synthesized in presence of alkali (Na, K, B, and P) impurities and under sulfur atmosphere to stabilize alpha-prime dicalcium silicate. The synthesized clinkers were characterized using x-ray diffractometry (XRD) to quantify the phases present using the Rietveld method. Preliminary results have demonstrated that adequate amounts of alpha-prime dicalcium silicate were stabilized in clinkers reaching about 87%wt. of total clinker composition. This is a promising step towards the commercial production of low-carbon high-strength cement formulations.

UTILIZING THE MOLECULAR SIMULATION DESIGN FRAMEWORK (MoSDeF) TO SCREEN SOFT MATTER SYSTEMS

Clare M^{c}Cabe
Department of Chemical & Biomolecular Engineering,
Vanderbilt University, Nashville TN
c.mccabe@vanderbilt.edu

Soft matter systems (those easily deformed at room temperature - e.g., liquids, polymers, foams, gels, colloids, and most biological materials) are ubiquitous in chemistry, but they pose particular computational challenges since the differences in potential energy between distant configurations are on the same order as the thermal motion, requiring time and/or ensemble-averaged data to be collected over long simulation trajectories for property evaluation. Furthermore, performing a molecular simulation of a soft matter system involves multiple steps, which have traditionally been performed by researchers in a “bespoke” fashion. The result is that many soft matter simulations published in the literature are not reproducible based on the information provided in the publication, and large-scale screening (as envisaged in the Materials Genome Initiative) of soft materials systems is a formidable challenge.

To address the issues of reproducibility and automation needed to enable computational screening, we have been developing the Molecular Simulation and Design Framework (MoSDeF, http://mosdef.org) software suite. MoSDeF includes the open-source mBuild (https://github.com/mosdef-hub/mbuild), Foyer (https://github.com/mosdef-hub/foyer) and GMSO (https://github.com/mosdef-hub/gmso) packages. We will introduce MoSDeF and its capabilities in this presentation. We will also show how, by combining MoSDeF with the Glotzer group’s Signac-flow workflow manager (https://bitbucket.org/glotzer/signac-flow), we can facilitate screening of soft matter systems over chemical/structural parameter spaces.

Specifically, results will be presented for the lubrication of nanoscale devices featuring surfaces functionalized by monolayers in sliding contact. Using MoSDeF, a combinatorial screening study was performed to explore tens of thousands of unique monolayer films. While this approach enables us to determine systems with favorable properties more rapidly than could be accomplished through experiment, the screening process still requires a significant amount of time and computing resources. Here, we illustrate the value of coupling MD simulations with machine learning (ML) in order to guide the screening process and reduce the simulations needed in order to optimize system designs. The ML-derived structure-property relations then enable screening of hundreds of thousands of candidate monolayer films, since the structure-property relation requires trivial computational resources.

Catalysis and Polymers

ASSESSING THE EFFECT OF HALLOYSITE CLAY AND ITS TREATMENT AS AN EFFECTIVE NICKEL SUPPORT FOR DRY REFORMING OF METHANE

Dema Almasri,[1] **Alessandro Sinopoli,**[1] **Ahmed Abotaleb**[1]

[1] *Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. Box 34410, Qatar Foundation, Doha, Qatar*

E-mail: delmasri@hbku.edu.qa

Dry reforming of methane (DRM) has recently received wide attention due to its outstanding performance in the reduction and conversion of CH_4 and CO_2 to syngas (H_2 and CO). From an industrial perspective, nickel (Ni) supported catalysts have been deemed as the most suitable catalysts for DRM due to their low-cost and high activity, compared to noble metal catalysts. However, a downside of nickel catalysts is their high susceptibility to deactivation due to coke formation and sintering at high temperatures. Using appropriate supports and preparation methods play a major role in improving the activity and stability of Ni supported catalysts. In this study, halloysite nanotubular (HNT) clay is utilized as a support for Ni. Clays are abundant, low-cost materials that can be easily modified. HNT clay has a unique tubular structure with a silica exterior and alumina interior. In this study, efforts are made to activate the surface of HNT with acids (HNO_3 and H_2SO_4) and alkaline treatment ($Na_2CO_3 + NaNO_3$) prior to Ni doping in order to observe the effect of support treatment on the stability, activity and longevity of the catalyst. In this work, 10 wt.% Ni catalysts on raw HNT, acid treated HNT, and alkaline treated HNT supports were prepared via the wet impregnation method. A detailed characterization of the catalysts is conducted by X-ray diffraction (XRD), BET surface area analysis, transmission electron microscopy (TEM), and X-ray photo electron spectroscopy (XPS) techniques. Preliminary results depict the surface area of the Ni doped on the H_2SO_4 treated HNT (SA > 144 m^2/g) to be more than 2 folds greater than that on raw HNT (53.6 m^2/g) and on the HNO_3 treated HNT (67.4 m^2/g). Electron microscopic images demonstrate an obvious alteration in the structure of HNT after treatment, and elemental mapping shows a uniform distribution of Ni throughout the support. The morphology, chemical structure, and performance testing of the developed catalysts are presented.

COMBINATORIAL SYNTHESIS OF HETEROCYCLIC COMPOUNDS USING NON-ASYMMETRIC ORGANOCATALYSTS

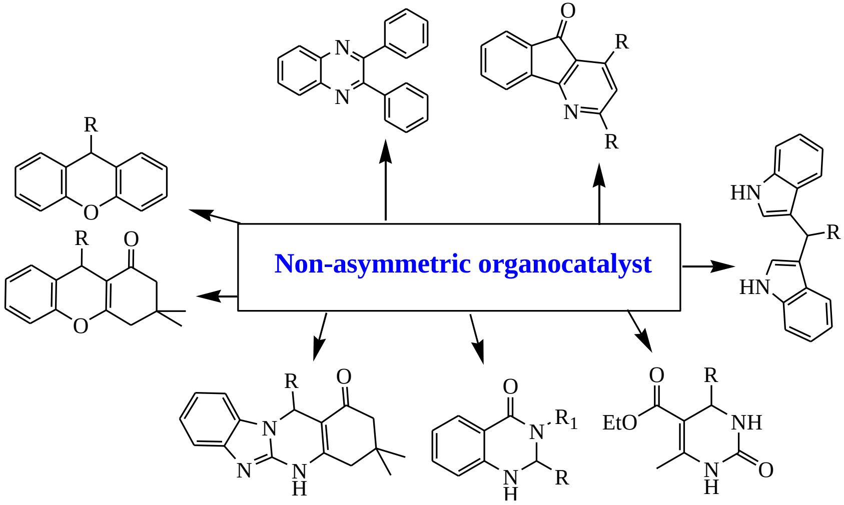
Samad Khaksar

School of Science and Technology, The University of Georgia, Tbilisi, Georgia

In the past 20 years, organocatalysis has arisen as a robust procedure in organic chemistry for making/the formation of carbon-carbon and carbon-heteroatom bonds [1]. Recently, organocatalytic reactions affording achiral compounds have received significant attention as a low-cost, non-toxic, readily available methodology that affords the relating products with excellent selectivity in high yields [2].

Heterocycles are widely investigated for their various biological properties [3], such as GABAA receptor ligands, topoisomerase IIa inhibitors, kinase inhibition, anti-HIV, anti-proliferative agents, antimalarial, anti-inflammatory, and anticancer.

The proposed work discusses our recent achievements in using non-asymmetric organocatalysts to synthesize highly functionalized heterocycles [4, 5]. [(Scheme1)



Scheme 1. Synthesis of heterocyclic compounds using non-asymmetric organocatalyst

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Development of active and stable Ni-based catalysts for CO_2 reformation of CH_4

[a]Sardar ali, [b]Dharmesh kumar, [a]Muftah El-Naas

[a]Gas processing center, Qatar University, Doha, Qatar
[b]Qatar Shell research and technology center

Abstract:

Ni-based catalysts supported over lanthana (La_2O_3), zirconia (ZrO_2) and alumina (Al_2O_3) were synthesized by solution combustion synthesis (SCS) method. The calcined catalysts were characterized by the analytical techniques of temperature programmed reduction (H_2-TPR), transmission electron microscopy (TEM) and X-ray diffraction (XRD) techniques. The effects of support on the performance of Ni-based catalysts in the CO_2 reformation of methane was then investigated. The results indicated that the nature of catalyst support significantly influenced the interactions and nature of NiO species. This lead to a remarkable difference in the reduction behavior and catalytic activity of the tested catalysts.

The alumina supported 5wt%Ni/Al_2O_3 catalyst exhibited superior catalytic activity and stability during the DRM compared to the Ni/La_2O_3 and Ni/ZrO_2 catalysts. During T.O.S. stability testes, the Ni/La_2O_3 catalyst started with an initial high CH_4 (~95.3%) conversion than that of the Ni/Al_2O_3 catalyst (~88.7%) but the Ni/La_2O_3 catalyst deactivated severely, by contrast the Ni/Al_2O_3 stayed active. The zirconia supported Ni catalyst exhibited the least activity. This catalyst did not show any activity at an operating temperature below 800^{o}C. The higher catalytic activity and stability of the Ni/ Al_2O_3 was attributed to the formation of uniformly distributed nickel aluminate nano-crystallites together with nickel oxide.

Keywords: metal-support interactions, nickel nanoparticles, methane reformation

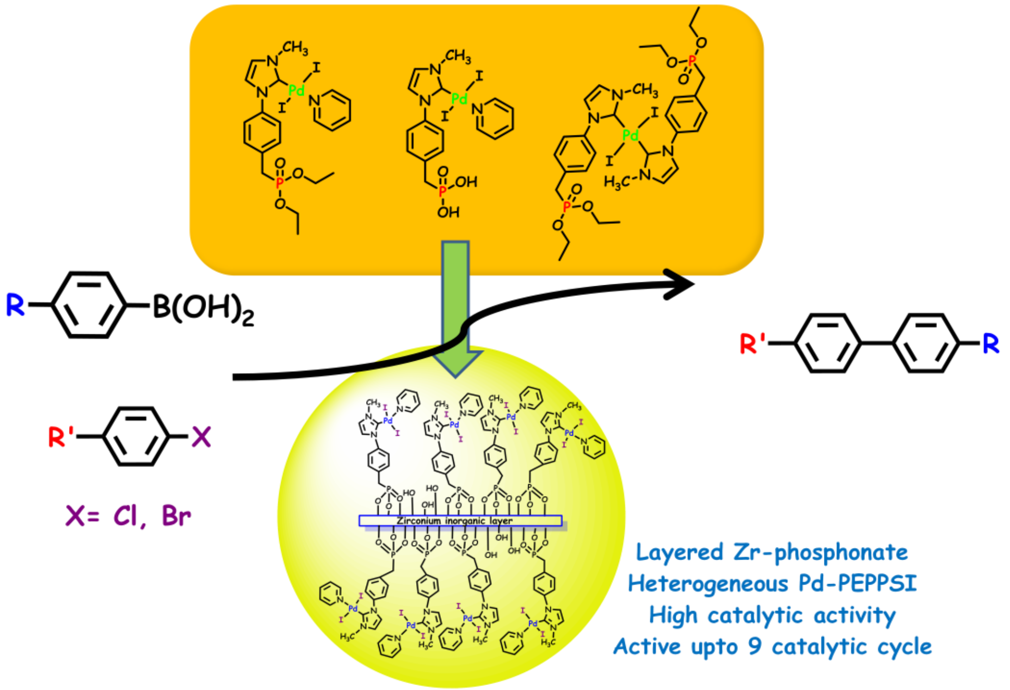
Heterogenization of a Pd-NHC catalyst and comparative study of their catalytic activity toward Suzuki cross coupling reaction

Bagmita Bhattacharyya, Nayanmoni Gogoi*

Department of Chemical Sciences, Tezpur University, Assam, India

Email: ngogoi@tezu.ernet.in

Catalytic reactions are important class of reaction for synthesis of material for pharmaceutical and industrial importance. About 95% of the industrial reactions are carried out catalytically, while 18% of the reactions involved are C-C or C-heteroatom coupling reactions. Palladium being the catalyst for most of these coupling reactions, various catalytic systems of palladium has been reported till date. Pd-N heterocyclic carbene (Pd-NHC) is one such systems having superiority in terms of activity, efficiency and stability than the other catalysts like nanoparticles and Pd-phosphine based ligand systems. In view of the above advantages in this work we have explored the Suzuki cross coupling reaction with aryl chloride and boronic acid, using a set of three new homogeneous Pd-NHC systems. But the lack of reusability associated with the homogeneous systems has pushes the research towards development of heterogeneous systems having reactivity and selectivity comparable to their homogeneous counterpart. Therefore, success achieved by using Pd-NHC heterogeneous systems is significantly inspiring attributed to their strong M-NHC bond, which helps in stabilization of catalyst during cycles and prevention of contamination of residual palladium in products. Thus using the reported homogeneous catalytic system as starting ligand a heterogeneous Pd-NHC system supported over Zr(IV)phosphonate was prepared and compared their catalytic activity for similar sets of reactions. The heterogeneous system showed high catalytic consistency and recyclability upto nine catalytic cycles.



LOW TEMPERATURE *IN SITU* POLYMERIZATION OF VINYL ACETATE THROUGH EMULSION GELS

Nazreen Zavahir[1], Madhubashini Maddumaarachchi[2]

[1]Department of Chemistry, University of Sri Jayewardenepura, Sri Lanka
[2]Department of Polymer Science, University of Sri Jayewardenepura, Sri Lanka
E-mail: nazreenzav@gmail.com

Emulsion gel polymerization has received immense attention as it allows free radical chain reactions at a reduced temperature to obtain polymers with higher molar masses. An *in situ* radical polymerization for a better conversion is possible with 2,2'-azobis(isobutyronitrile) (AIBN) initiator and fumed silica, which forms a three dimensional network with surfactant molecules to catalyze free radical polymerization at a good rate [1]. AIBN, which produces radicals at an elevated temperature (about 60 ˚C), complexes with surfactant to occur the polymerization comparatively at a reduced temperature.

This study aims to polymerize vinyl acetate (VAc) at a reduced temperature through an emulsion gel. Emulsion gel polymerization (EGP) of VAc was conducted at room temperature (RT), 40 and 60 ˚C using purified VAc, AIBN and cetyltrimethylammonium bromide (CTAB), and discovered about 90% conversion of VAc in 9 h at 40 ˚C. Further, The T_g of poly(vinyl acetate) (PVAc) polymerized in these emulsion gels with silica was higher (T_g = 41 ˚C) than those of PVAc made from bulk polymerization at 60 ˚C (T_g = 31℃) and the weight average molar mass (M_w) was also larger (M_w about 300 kg/mol) than those from bulk polymerization (M_w = 125 kg/mol). Increased M_w, T_g and lowered processing temperature for these composites could facilitate new applications for PVAc. Polymerization of VAc proceeded at a very low rate in the absence of surfactant even at a slightly elevate temperature of 60 ^{0}C. EGP of VAc was conducted using CTAB (cationic), sodium dodecylsulfate (SDS, anionic) or triton X-100 (non-ionic). The order of conversion of VAc was CTAB > triton X-100 > SDS, due to different degree of inhibition occurred. Lengthy PVAc chains formed in the presence of SDS, showed higher T_g, M_w and polydispersity (42 ^{o}C, 376 kg/mol, 2.70) for bulk PVAc. PVAc from PVAc/silica/triton X-100 resulted relatively a low M_w (267 kg/mol) with a narrow polydispersity (2.23).

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MATERIAL CHEMISTRY PROSPECTS OF TRIAZAPHOSPHOLE DERIVATIVES AND TRIAZOLE-DERIVED CARBENES

Rajendiran Marimuthu[a], Martin Papke[b], Christian Müller[b] and **Ramaswamy Murugavel***[,a]

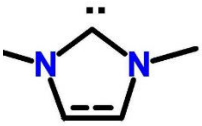
[a]*Department of Chemistry, Indian Institute of Technology Bombay (IIT Bombay), Mumbai-400076, India,*

[b]*Freie Universität Berlin, Germany*

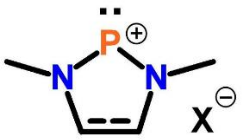
E-mail: marimuthusrs@gmail.com

Recent years, the low-coordinate organo-phosphorus compounds have regained noticeable interest due to their unusual electronic and steric properties. Triazaphospholes plays a vital role in the coordination and materials chemistry and importantly in stabilizing the low coordinate metal complexes; these triazaphospholes used for various application like organic light emitting diodes (OLEDs) sensing materials, light-emitting organophosphorus containing molecular materials and activation of small molecules such as H_2, NH_3, CO_2, alkenes and ketones.

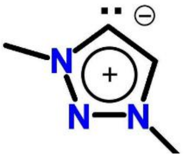
Here bulky aryl-azides have been synthesized from the corresponding primary amines. The reaction of these aryl azides with phosphaalkynes yields 3H-1,2,3,4-triazaphosphole derivatives. Representative triazaphospholes can be selectively alkylated with variant of Meerwein's reagent on the most nucleophilic nitrogen atom to yield stable 1,2,3,4-triazaphospholenium cations. These compounds were characterized bysolution NMR (^{1}H, ^{13}C, ^{31}P, ^{19}F and ^{11}B NMR), mass spectrometry and single crystal X-ray diffractions.



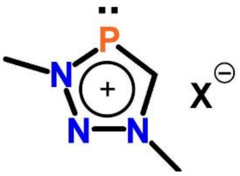
Carbene



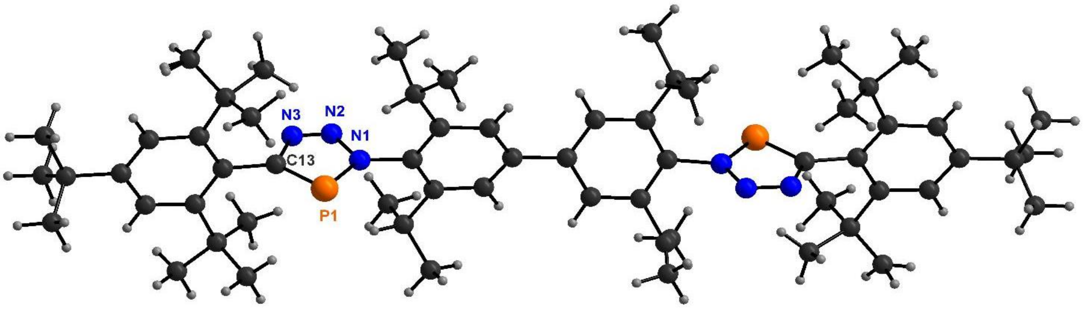
1,3,2- diazaphospholenium cation



1,2,3-triazolylidene



1,2,3,4-triazaphospholenium salt



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MODELLING OF CATALYST DEACTIVATION ON THE DRY REFORMING OF METHANE (DRM) USING THE GENERALIZED POWER LAW EXPRESSION (GPLE)

N. A. Mohamed[1], H. A. Choudhury[2], S. Afzal[1], A. Chatla[1], N. O. Elbashir[1,2]

[1] *Chemical Engineering Program, Texas A&M University at Qatar, Doha, Qatar*

[2] *Petroleum Engineering Program, Texas A&M University at Qatar, Doha, Qatar*

E-mail: nosaiba.am28@gmail.com

One of Qatar's major challenges, "The World Capital in Natural Gas Processing," is reducing the emissions of gas processing plants and improving the product's carbon footprint. Therefore, Qatar has invested heavily in building one of the world's largest gas-to-liquid (GTL) plants of enhanced energy and mass integration that follows stringent environmental regulations. Nevertheless, Qatar is still leading the world in carbon dioxide emissions per capita, which negatively impacts the carbon footprint of its GTL plant's ultra-clean fuels, and other products. One of the proposed solutions to reduce GTL product's carbon footprint is the dry reforming of methane (DRM) technology that utilize two major greenhouse gases (methane and carbon dioxide) to produce syntheses gas as follow:

DRM reaction: $\mathrm{CH_4 + CO_2 \rightarrow 2CO + 2H_2}$ $\quad \Delta H^{\circ}_{298K} = 247\,\frac{\mathrm{kJ}}{\mathrm{mol}}$ (1)

Methane decomposition: $\mathrm{CH_4 \leftrightarrow C + 2H_2}$ $\quad \Delta H^{\circ}_{298K} = 75\,\frac{\mathrm{kJ}}{\mathrm{mol}}$ (2)

Boudouard reaction: $\mathrm{2CO \leftrightarrow CO_2 + C}$ $\quad \Delta H^{\circ}_{298K} = -171\,\frac{\mathrm{kJ}}{\mathrm{mol}}$ (3)

Revers water gas shift (RWGS) reaction: $\mathrm{CO_2 + H_2 \rightarrow CO + H_2O}$ $\quad \Delta H^{\circ}_{298K} = 41\,\frac{\mathrm{kJ}}{\mathrm{mol}}$ (4)

However, the DRM reaction (Rxs1) also suffers from severe catalyst deactivation problems related to the multiple carbons produced in the side reaction (Rxs2 and 3). To better understand the deactivation mechanisms of the nickel-based catalyst because of these reactions, a semi-empirical method was used to model the catalyst deactivation mechanism. A Generalized Power Law Expression (GPLE) [1] model was used to fit the activity profile and predict the catalyst deactivation mechanism as follow:

$-\frac{da}{dt} = k_d\, P(c)_d\, a^d + constant$; where a is the normalized activity, $\mathrm{k_d}$ is deactivation rate constant.

Two sets of catalytic systems were used in the study. The first set is the monometallic (10%Ni/γ-Al_2O_3) and bimetallic (10%Ni_8Cu_1/γ-Al_2O_3) catalyst to study the effect of adding Cu promoter in the catalyst activity. The second set is the commercial catalyst (Riogen) at two different temperatures (650 and 550°C). The GPLE model fits the experimental data with regression factor (R^2) ranging between 0.95 and 0.99. Also, the first and second-order GPLE model was used to deconvolute the activity profile based on the deactivation mechanism for all the catalyst systems. In the commercial catalyst (Riogen), the model results indicate that at 550 °C, the percent of activity lost from carbon deposition is higher than the percent at 650 °C, which agrees with literature reports. In the bimetallic and monometallic catalysts, the results indicate that the rapid deactivation of monometallic catalyst is primarily due to significant coke formation. In contrast, the bimetallic catalyst experienced minimal deactivation due to both particle sintering in the initial stages followed by coke formation.

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PACKED BED MICROREACTOR AS A TOOL FOR TESTING OF METAL-ORGANIC FRAMEWORKS BASED CATALYST

Anchu Ashok[1], Wenmiao Chen[2], Madrahimov Sherzod[2], Ma'moun Al-Rawashdeh*[1]

[1]*Chemical Engineering Department, Texas A&M University at Qatar, Doha, Qatar*
[2]*Chemistry Department, Texas A&M University at Qatar, Doha, Qatar,*
E-mail: mamoun.al-rawashdeh@qatar.tamu.edu

Compared to batch reactor testing, flow chemistry and microreactors showed superior performance to accelerate the discovery and development of new chemical processes, improve safety, and are ideal when the available amount of chemicals and catalysts are limited. All these are desired features for the screening and testing of novel catalytic materials. Metal-Organic Frameworks or MOF's is a new class of heterogeneous catalysts with tremendous opportunities as they can be atomically designed with modular properties, functionalized with specific sites or specific assets. The majority of available MOF's are still at the laboratory stage, and mainly available in the form of powder typically in smaller quantities at the grams scale.

Introducing solid particles in microreactors is not a straightforward task especially when it comes to heterogeneous catalysts testing and obtaining kinetic data. In this work, different MOF's catalysts were tested in capillary microreactors for liquid-solid and gas-liquid-solid type reactions of C-C coupling, hydrolysis, and semi-hydrogenation[1,2]. Testing was executed for different in-house synthesized MOF's types that have different porosity, crystal sizes, functionality, and incorporated metal nanoparticles. Catalysts were tableted and sieved to make a different range of particle sizes that were loaded in the capillary microreactor. Reaction testing was carried out at different operating conditions. Opportunities and limitations for this approach of catalysts packing and testing will be presented in this work.

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PROPERTIES AND PERFORMANCE OF OIL-SORBENT FILMS PREPARED FROM WASTE POLYOLEFINS AND THEIR BLENDS

Samra Sajjad[1], Adriaan S. Luyt[1]*, Ahsan K. Hafeez[1], Gordon Mckay[2], Junaid Saleem[2]*, Abdul Shakoor[1]

[1] Center for Advanced Materials, Qatar University, Doha, QATAR

[2] College of Science and Engineering, Hamad Bin Khalifa University, Doha, QATAR

Email: samra.sajjad@qu.edu.qa

** Corresponding authors (aluyt@qu.edu.qa, jsaleem@hbku.edu.qa)*

This paper reports on the thermal and oil absorption properties, as well as the morphologies, of films prepared from different waste polyolefin blends. Salt was mixed into these blends and then extracted in water after film formation in order to produce porous films that could absorb oil from an oil/water mixture. Complete differential scanning calorimetry (DSC) analysis of all the samples showed co-crystallization of certain polymers in the blends, as well as incomplete salt extraction of the salt from some of the blends. A combination of atomic force microscopy (AFM) and SEM showed the presence of micro-sized pores, as well as differences in surface roughness between the films, and this was directly related to oil uptake efficiency. When analyzing the oil absorption capacities of the different blend films after salt extraction, it was found that the LDPE/HDPE/PP blend film most effectively absorbed the oil. Scanning electron microscopy (SEM) pictures showed the presence of a small number of salt crystals in the film after salt extraction, and it was found that the salt crystals had an observable affinity for the oil. Contact angle results showed that this blend also was the most oleophilic of all the investigated blends. The effectiveness of this blend in absorbing the oil can therefore be explained by a combination of the presence of pores in the film, and the attraction that both the polymer blend and the salt crystals have for the oil.

Rh(I)-BASED METAL ORGANIC FRAMEWORKS FOR SELECTIVE CO-DIMERIZATION OF OLEFINS AND TERMINAL ALKYNES

Veeranna Yempally[1], Wenmaio Chen[2], Hong-Cai Zhou[2], Sherzod Madrahimov[1]

[1] Chemistry Department, Texas A&M University at Qatar, Doha, Qatar.
[2] Chemistry Department. Texas A&M University, College station, U.S.A.
E-Mail: veeranna.yempally@qatar.tamu.edu

Metal organic frameworks (MOFs) have potential application as sustainable catalysts in various important organic transformations, such as ethylene olegomerization, polymerization, and also for the homo-dimerization of olefins, and alkynes. [1]. However, there are very few reports concerning the co-dimerization of olefins with alkynes employing MOFs as catalysts. The co-dimerization process is widely used in polymer industry to produce monomer precursors for synthetic rubber production, and also in the pharmaceutical industry to synthesize active bio-molecules [2]. Homogeneous catalysts based on Rh, and Ru have been explored previously for efficient co-dimerization of olefins and terminal alkynes [3]. However, selectivity in exclusive production of 1,3-butadienes is scarcely reported. The superior catalytic activity of single site active catalysts immobilized on MOF’s compared to analogues homogeneous catalysts is well established [4]. The present study is aimed at exploring the catalytic activity of Rh(I) metal immobilized on UiO-66-PPh_2 MOF, and UiO-66-PNP-Ph_2 MOF for the selective co-dimerization of olefins with terminal alkynes to produce 1,3-butadienes. The post-synthetic metalation of UiO-66-PPh_2 MOF with the variety of Rh(I) metal precursor afforded three different catalysts containing Rh(I) cationic complexes immobilized on UiO-66-PPh_2 MOF. The primary objective of the present study is to explore the catalytic activity and selectivity of cationic Rh(I) metal-based MOFs and comparing the catalytic activity in selective synthesis of 1,3-butadiene. The catalysts morphology, stability, and elemental distribution were characterized with the help of XRD, TGA, and SEM-EDX analysis respectively. Herein, we present the preliminary results obtained in the catalytic co-dimerization of olefins with terminal alkynes employing MOF catalysts containing cationic Rh(I) metal on the surface.

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SINGLE ION CONDUCTING BLOCK COPOLYMERS

Yossef A. Elabd[1, 2]

[1]Office of Research, The Texas A&M University System, College Station, TX 77840
[2]Department of Chemical Engineering, Texas A&M University, College Station, TX 77843

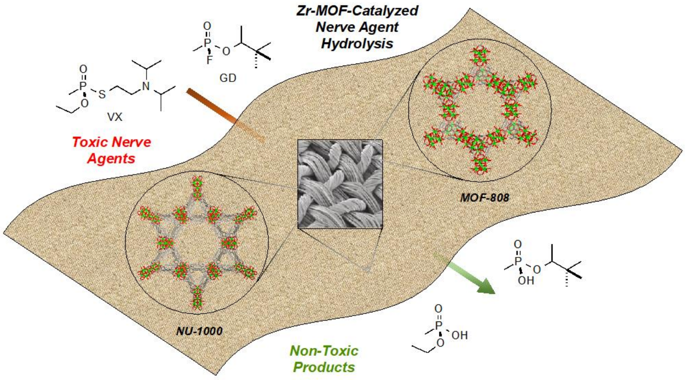
Single ion conducting block copolymers can possess the orthogonal properties of high ion conduction and high mechanical strength within robust thin films and therefore have been explored for their use in batteries and fuel cells. Additionally, the morphology type, periodicity, and phase separation strength of the self-assembled nanostructures that form within single ion conducting block copolymers and their subsequent impact on ion conduction have been a subject of great interest. In this work, the ion transport properties and morphology of a variety of single ion conducting diblock copolymers and multiblock polymers synthesized in our laboratory will be presented. Specifically, a fundamental understanding of transport-morphology relationships in these materials as a function of various chemistries and chain architectures will be examined. The application of these materials as solid-state separators for lithium-ion batteries and membranes for both proton exchange membrane fuel cells and alkaline exchange membrane fuel cells will also be discussed.

Smart and Programmable Sponges for protection From Bench to Market

Omar K. Farha

Northwestern University

This talk will focus on metal–organic frameworks (MOFs) from basic research to implementation and commercialization. MOFs are a class of porous, crystalline materials composed of metal-based nodes and organic ligands that self-assemble into multi-dimensional lattices. In contrast to conventional porous materials such as zeolites and activated carbon, an abundantly diverse set of molecular building blocks allows for the realization of MOFs with a broad range of properties. We have developed an extensive understanding of how the physical architecture and chemical properties of MOFs affect material performance in applications such as catalytic activity for chemical warfare agent detoxification.



SnO_2-CuO EMBEDDED Ni-FOAM CATALYST FOR EFFICIENT CONVERSION OF CO_2 INTO FORMATE.

Haseena Onthath,[1] **Mansoor Al-Shamri,**[2,3] **Sifani Zavahir,**[1] **Ahmed Khodary,**[3]

Dong Suk Han[1, 4]

[1]Center for Advanced Materials (CAM), Qatar University, Doha 2713, Qatar
[2]University of Bradford, Richmond Rd, Bradford BD7 1DP, United Kingdom
[3]Qatar Shell Research & Technology Center, Doha 3747, Qatar
[4]Department of Chemical Engineering, College of Engineering, Qatar University, Qatar
Email: haseena@qu.edu.qa

The effective conversion of CO_2 into various fuels and chemicals has become a major challenge for efficient carbon neutralization of the synthetic production chain. Formate, which is widely used as a hydrogen storage vector and a precursor to high value-added products, has attained considerable interest in recent years. So, this study aims to construct an electrocatalyst and system that can selectively convert CO_2 to formate. However, electrocatalysts to date suffer from various inconsistencies in that they are good platforms for effective and selective CO_2 reduction. Here, we demonstrated the improved selectivity and activity of SnO_2 over CO_2 reduction into formate tailored by alloying CuO nanoparticles. From the theoretical and experimental studies, we realized that the incorporation of CuO particles can significantly enhance the electrocatalytic behavior of SnO_2-CuO nanocomposite. Furthermore, here we used porous Ni-foam as catalyst support that provides a large surface area which contributes to facile delocalization during CO_2 reduction reaction. The selection of K_2SO_4 as an electrolyte also favors formate production in such a way that the presence of sulfur enhances the activation of H-species, which can readily react with water to form formate. Among the different ratios of SnO_2 and CuO studied (1:1, 1:3, 3:1), the catalyst mixture in the same ratio (1:1) showed better electrocatalytic performance. It was confirmed that the formate production ability of the SnO_2-CuO nanocomposite is further increased due to the synergistic electrocatalytic interactions between SnO_2 and CuO.

STEREOCONTROLLED POLYMERIZATIONS BASED ON OLEFIN METATHESIS

Quentin Michaudel[1,2]

[1]Department of Chemistry, Texas A&M University, College Station, TX 77843

[2]Department of Materials Science & Engineering, Texas A&M University, College Station, TX 77843

E-mail: quentin.michaudel@chem.tamu.edu

Since the development of the first industrial processes capitalizing on ring-opening olefin metathesis polymerization (ROMP) almost 50 years ago, the continuous invention of new families of homogeneous catalysts and olefinic monomers has enabled the precise synthesis of macromolecules with ever-increasing complexity. This powerful synthetic manifold allows the preparation of soft materials with tailored molecular structures and tunable physicochemical properties for applications ranging from healthcare to organic semiconductors. The Michaudel laboratory is developing synthetic methods based on olefin metathesis to prepare conjugated materials and polyalkenamers that were previously unattainable. This presentation will focus on the development of stereocontrolled polymerization systems that allow the practitioner to dictate the ratio of *cis* (*Z*) or *trans* (*E*) double bonds throughout the polymer backbone. This structural parameter has been shown to drastically impact the thermal, mechanical, and optoelectronic properties of polymers, but general and efficient methods allowing the synthesis of stereodefined materials are scarce. The first part of the talk will highlight the potential of stereoretentive olefin metathesis to access all-*cis* poly(phenylene vinylene)s with exquisite stereoselectivity and desirable living characteristics [1]. The influence of monomer structure and dithiolate Ru-carbene catalysts over the rate of polymerization and the properties of the synthesized polymers will be discussed [2]. Finally, the design of a stereocontrolled acyclic diene metathesis (ADMET) process through careful optimization of monomer, catalyst, and reaction conditions will be presented [3]. This versatile reaction manifold allows the preparation of polyalkenamers with diverse structures and predictable *cis*:*trans* ratios. Examples of polyesters, polycarbonates, polysulfites, and polyethers will illustrate the potential of this method to precisely tune the properties of soft materials.

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SYNTHESIS AND CATALYTIC APPLICATION OF NOVEL CYCLIC AND BICYCLIC (ALKYL)(AMINO) CARBENE – TRANSITION METAL COMPLEXES

Márton Nagyházi,[1] Robert Tuba[1]

[1]Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar tudósok körútja 2., 1519 Budapest, P.O. Box 286. Hungary

E-mail: nagyhazi.marton@ttk.hu

Cyclic carbene ligands show remarkable development in the past decades. Bearing better electronic properties than NHCs, novel cyclic (CAAC) and bicyclic (alkyl)(amino)carbenes (BICAAC) are synthetized. The new carbenes with varying functional groups were applied as ligands in olefin metathesis (Grubbs-type Ru complexes)[1,2] and C-C cross-coupling reactions (PEPPSI-type Pd complexes)[3].

In situ generated CAACs featuring *tertiary* amine groups were reacted with Grubbs and Hoveyda-Grubbs 1st generation complexes, yielding CAAC-analogues of the 2nd generation equivalents *via* phosphine-carbene exchange. Upon *N*-alkylation, *quaternary* ammonium groups were formed, allowing the application of complexes in polar, even protic media for catalytic reactions. Olefin metathesis reactions (RCM, isomerization, ROMP, ADMET polymerization) were successfully catalyzed in methanol using as low as 0,05 mol% CAAC-Ru catalyst loading. [1]

The BICAAC analogues of the CAAC ligands were prepared in a similar synthetic manner. The *N*-aryl moiety on the BICAAC system was varied by changing the *ortho*-positioned alkyl groups' size, and also *tertiary* amine (dimethylamino) group was applied as substituent. The novel ligands were able to form complexes with Grubbs and Hoveyda-Grubbs 1st generation complexes *via* phosphine-carbene exchange. Five such complexes were synthetized and characterized by XRD. Interestingly, the new BICAAC-Ru complexes show high, but latent catalytic activity in olefin metathesis: their activation limit is between 50 and 75 °C [2].

Reacting the above mentioned BICAAC ligands with *bis*(pyridine)$PdCl_2$, the exchange of only one pyridine ligand was observed yielding the corresponding PEPPSI-type Pd-complexes [$PdCl_2$(pyr)(BICAAC), five examples, two XRD structures]. Similarly to their NHC-analogues, they found to be able exceptional precatalysts for Mizoroki-Heck coupling reactions. [3]

A general observation, that bulkier BICAAC ligands tend to form less reactive catalytic species (*ortho* Me > Et > iPr at Ru-cat. olefin metathesis; 4-positioned Me > iPr at Pd-cat. Heck reactions). Meanwhile, the presence or absence of the electron-donating dimethylamino group has no serious effect either the complex characteristics, or the catalytic activity in any cases.

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Synthetic Peptides as Inhibitors for Efflux Pumps of Multidrug-Resistant Bacteria

Abeer I. M. Obeidat,[1] Da’san M. M. Jaradat,[1,*] Nehaya Al-Karablieh[2]

[1]Department of Chemistry, Faculty of Science, Al-Balqa Applied University, P.O. Box 19117, Al-Salt, Jordan,

[2] Faculty of Agriculture, Department of Plant Protection, The University of Jordan, Amman, Jordan; and Hamdi Mango Center for Scientific Research, The University of Jordan, Amman, Jordan

*Author for correspondence: Da’san M. M. Jaradat, dasan.jaradat@bau.edu.jo

The rapid increase in multidrug-resistant (MDR) bacteria emergence has presented a serious challenge that motivates researchers to synthesize new agents including efflux pump inhibitors to tackle this growing challenge. In this research, four artificial 12-mer and 8-mer peptides were synthesized by solid-phase peptide synthesis (SPPS) strategy using Rink Amide AM resin. Purity of these peptides was determined by HPLC and their structures were confirmed by LC-MS/MS. Synergistic effect of these peptides in the presence of various antibiotics and chemicals was investigated on MDR bacteria. All synthetic peptides decreased the MIC values against the selected AcrAB-TolC substrates by 4 to 8 folds in *E. coli* TG1 and 4 to 16 folds in *E. amylovora* 1189 suggesting promising synergistic effect. Activity of these synthetic peptides as inhibitors of drug-efflux pumps belonging to *E. coli* TG1 and *E. amylovora* 1189 bacteria was investigated by intercellular ethidium bromide (EtBr) accumulation assay. All of which showed promising inhibition activity at different concentrations ranging from 12.5 μg/mL to 100 μg/mL that was comparable to that of a reference efflux pump inhibitor (EPI). The optimal inhibitory activity was at 100 μg/mL.

Poster Session on General Topics in Chemistry and Chemical Engineering

ADSORPTION CHARACTERISTICS OF PRISTINE AND MAGNETIC OLIVE STONES BIOCHAR WITH RESPECT TO CLOFAZIMINE

Marwa El-Azazy,[1] Iman Nabil,[1] Siham S. Hassan,[1] Ahmed S. El-Shafie[1]

[1]*Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University,*
Doha 2713
E-mail: marwasaid@qu.edu.qa

Olive stone biochars (OSBC), both pristine and following magnetization (MAG–OSBC), were utilized as eco-friendly and cost-effective sorbents for the antituberculosis, clofazimine (CLOF). Morphologies, textures, surface functionalities, and thermal stabilities of both adsorbents were explored using SEM, EDX, TEM, BET, FT-IR, Raman, XRD and TGA analyses. SEM analysis showed meso and macroporous surfaces. BET data showed that the MAG–OSBC possesses a larger surface area (33.82 m^2/g) and pore volume. Batch adsorption studies were conducted following the experimental scenario of Box–Behnken (BB) design. The adsorption efficiency of both adsorbents was evaluated in terms of the % removal (%R) and the sorption capacity (qe, mg/g). Dependent variables (%R and qe) were maximized as a function of four factors: pH, sorbent dose (AD), the concentration of CLOF ([CLOF]), and contact time (CT). A %R of 98.10% and 98.61% could be obtained using OSBC and MAG–OSBC, respectively. Equilibrium studies indicated that both Langmuir and Freundlich models were perfectly fit for adsorption of CLOF. Maximum adsorption capacity (q_{max}) of 174.03 mg/g was obtained using MAG–OSBC. Adsorption kinetics could be best illustrated using the pseudo-second-order (PSO) model. The adsorption–desorption studies showed that both adsorbents could be restored with the adsorption efficiency being conserved up to 92% after the sixth cycles [1].

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AN ASSESSMENT OF DEVELOPED THERMOCHROMIC SOLAR FILMS FOR ENERGY CONSERVATION

Aysah Melhim[1], Noor Mubark[1], Dr. Mohammed Al-Hashimi[2], Dr. Sarbajit Banerjee[3]

[1]Deparment of Chemical Engineering, Texas A&M University, [2]Department of Science, Texas A&M University at Qatar, [3]Department of Chemistry, Texas A&M University

Email: aysha.melhim@qatar.tamu.edu

Energy consumption has become directly associated with buildings. According to the United Nations, it is estimated that buildings contribute by 30-40% of the worldwide energy consumption. The consumption of energy has increased due to urbanization in the past 20 years. Heating, cooling, in addition to external and internal heat gains are, primarily, the source of energy consumption in buildings. Solar heat gains and losses occur through several components of the buildings. For instance, the use of glass windows for indoor lighting. This research aims to assess developed thermochromic nanocomposite films that have been produced through the annealing of Vanadium Dioxide (VO2) nanocrystals within Silicon Dioxide (SiO2) shells. The nanocomposite solar films can spectrally select and dynamically tune control over the visible and infrared regions of the solar spectrum, allowing for control of the desired lighting and solar heat gain. The mathematical model will be built based on a conventional Qatar building (offices, villas, etc.). The control of the light and heat will, consequently, lower energy consumption for heating and cooling in buildings.

An ICP-MS Study on Metal Content in Biodiesel and Bioglycerol Produced From Heated and Unheated Canola Oil

Rukayat S. Bojesomo [1], *Dr. Abhijeet Raj* [2], *Mohamed I. Ali* [3],*Sasi Stephen* [1], *Mirella Elkadi* [1*]

[1] Department of Chemistry, College of Science, Khalifa University, P.O Box: 127788, Abu Dhabi, UAE. [2] Department of Chemical Engineering, College of Engineering, Khalifa University, P.O Box: 127788, Abu Dhabi UAE. [3] Department of Mechanical Engineering, College of Engineering, Khalifa University, P.O Box: 127788, Abu Dhabi, UAE.

Email: (M.E.). mirella.elkadi@ku.ac.ae

(R.B.) 100059967@ku.ac.ae

(A.R.) abhijeet.raj@ku.ac.ae

(M. A.) mohamed.ali@ku.ac.ae

(S.S.) sasi.stephen@ku.ac.ae

Abstract

The exorbitant cost associated with biodiesel production has been the major drawback to the commercialization of biodiesel. Reducing the cost of production by utilizing readily available, low-cost oil feedstock such as waste oil will equally reduce the cost of biodiesel production as well as address the issues of waste oil disposal around the globe. However, heating the oil at a high temperature leads to changes in the trace metal level of the oil and the biodiesel and bioglycerol produced from such oil. This also results in an elevated amount of free fatty acid (FFA) that can lead to a decrease in the biodiesel conversion and yield due to the formation of soap and water, which requires acid pretreatment, especially when an alkali catalyst is employed. In this regard, central composite design (CCD) based response surface methodology (RSM) analysis and conventional single factor optimization were applied to determine the relationship between methanol to oil molar ratio (M/O ratio), catalyst concentration (catalyst wt. %), and reaction time as independent variables and the optimum conditions for the maximum yield of biodiesel and bioglycerol production from unheated and heated canola oil at different temperatures (190 ºC and 240 ºC) for two hours. Also, the effects of heating temperature on the trace metal levels of the unheated and heated canola oil and their corresponding biodiesel and crude bioglycerol were studied using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). The optimum conditions for the highest biodiesel yield are a M/O ratio of 12:1, and a catalyst of 1.0 wt. %, and a reaction time of 60 minutes. With a molar ratio of 4.25:1, a catalyst wt. % of 2.93 wt. %, and a reaction duration of 119.15 minutes, crude bioglycerol will be produced in the range of 25% to 60%. Cu and Zn are high-concentration metals, whereas Pb, As, Se, and Zr, among other elements, are low-concentration elements in both unheated and heated oil feedstock and biodiesel and bioglycerol. Cs were not found in any of the samples analyzed. Thermal stress on canola oil was shown to have a remarkable and variable impact on the yield of biodiesel and crude bioglycerol and their trace metal levels.

Keywords: *Canola oil, Biodiesel, RSM, Trace metal, Waste oil*

AN IRON-CHROMIUM REDOX FLOW BATTERY TO PV-TIZE SOUTH AFRICA

Nico Mans,[1,*] Henning Krieg,[1] Derik van der Westhuizen,[1] Dolf Bruinsma.[2]

[1]Hydrometallurgy Group, Chemical Resource Beneficiation, North-West University, Potchefstroom 2520, South Africa
[2]Bruinsma Solutions, Potchefstroom 2520, South Africa
**Email: Nico.Mans@nwu.ac.za*

Due to the intermittent nature of renewable energy sources such as solar and wind energy, the development of suitable large-scale energy storage solutions (ESS) that can either be integrated into the existing power grid or be used off-grid, is essential. One of the current front runners to serve as an ESS for renewable energy is the redox flow battery (RFB) due to its high energy efficiency, extended lifetime, environmental friendliness and design flexibility.

Wide market penetration of RFB technology is yet to be accomplished mainly due to affordability and performance decay during cycling [1]. In the case of the all-vanadium RFB (VRFB), one of the main factors contributing to its high cost is the electrolyte price. To reduce the cost, alternative RFB electrolytes such iron-chromium could be considered, with both iron and chromium abundant and readily available [2].

South Africa is ideally suited for this development, considering its abundant sunshine and large chromium ore deposits. The two main disadvantages associated with the iron-chromium (ICRFB) is the potential higher capacity decay rate and the slightly lower storage capacity (compared to that of VRFB). To improve these two aspects and achieve optimal ICRFB performance requires a deep understanding of the effects of electrolyte components and additives on ICRFB performance.

Subsequently, it is the aim of this study to understand the effect of electrolyte components and additives on a lab scale ICRFB to determine the optimal electrolyte composition for peak ICRFB performance. From the results a significant improvement in terms of capacity retention and storage capacity could be achieved.

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AN UNEXPECTED MECHANISM FOR CO_2 HYDRATION PROMOTED BY NICKEL NANOPARTICLES, A COMBINED EXPERIMENTAL-COMPUTATIONAL APPROACH

Alessandro Sinopoli,[1] Ivan Gladich,[1] Ahmed Abotaleb,[1] Alaa Alkhateeb[1]

[1] *Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. Box 34410, Qatar Foundation, Doha, Qatar*

E-mail: asinopoli@hbku.edu.qa

Carbon Capture and Utilization (CCU) technologies certainly represent a promising way not only to reduce carbon dioxide impact on climate change, but also to convert CO_2 into added-value products/chemicals. The majority of CCU technologies, amine scrubbing and mineralization included, play around the dissolution of carbon dioxide in aqueous solution and the corresponding pH-dependent equilibria between CO_2(aq), carbonic acid (H_2CO_3), bicarbonate ion (HCO_3^-) and carbonate ion (CO_3^{2-}). Since the early studies on CO_2 dissolution, it was clear that the hydration (the multistep process responsible for the formation of carbonic acid) was the rate limiting step of the reaction, confirmed over the years by experimental and computational studies. In nature, CO_2 hydration reaction is catalysed by Carbonic anhydrase (CA), a zinc-based metalloenzyme able to accelerate the CO_2 hydration and dehydration rate. During the last decade, it has been suggested that nickel nanoparticles (NiNPs) can also propel the hydration of adsorbed CO_2 into carbonic acid. However, the catalytic effects of NiNPs on CO_2 hydration in water has been recently questioned in literature, also because a clear molecular understanding of the process is still missing. Here we present a combined experimental and computational (ab-initio molecular dynamics) study showing that, contrary to some common knowledge in literature, NiNPs does not catalyze the formation of carbonic acid in solution, but rather the CO_2 capture step. Indeed, the NiNP surface prefers to coordinate CO_2 rather than water to avoid a (negative) overcharging of the NP. The computational simulations are in agreement with the CO_2 loading measurements and the kinetics experiments. These results indicates that the apparent catalytic effect of NiNP in the carbonation of adsorbed CO_2 in aqueous solution is the results of an higher efficiency of the solution in capturing CO_2, rather than a catalytic conversion of CO_2 in carbonic acid on the surface of the NiNPs.

ANALYSIS OF ANTIMICROBIAL RESISTANCE PROFILES OF *ESCHERICHIA COLI* ISOLATED FROM PRE-HARVEST PRODUCE IN LEBANON

Sarah El Khechen[1], Rabi H. Mohtar [2], Issmat I. Kassem[3]

[1]Faculty of Agriculture and Food Sciences, American University of Beirut, Beirut, Lebanon

[2] Department of Biological and Agricultural Engineering, Texas A&M University, College station, TX, USA

[3]Food Science and Technology, Center for Food Safety, University of Georgia, Griffin, GA, USA

Antimicrobial resistance is an emerging global problem. Moreover, in Lebanon and other countries in the MENA (Middle East and North Africa) region, the lack of resources as well as underdeveloped infrastructure, and antimicrobial stewardship programs have further increased the spread of resistance in both human medicine and agriculture. Contamination with antibiotic resistant bacterial pathogens can happen across food systems; leading to transmission to humans via food and the food production environment. Of notable concern is the contamination of fresh produce with antibiotic resistant pathogens. Fresh produce can get contaminated via exposure to contaminated water and soil which are prevalent in low-income countries. Additionally, fresh produce are consumed without extensive processing which increases the risk to the public.

Data on the contamination of fresh produce are scant in Lebanon. Consequently, we aimed to study the prevalence of antibiotic resistant *E. coli* in pre-harvest produce in Lebanon. Sixty produce samples of different types (parsley, lettuce, radish, cucumber, and green onion) were collected from different regions in Lebanon. Seventy *E. coli* were isolated in total. Ten *E. coli* were colistin-resistant carrying the mobile colistin resistance gene (*mcr-1*) and seven of these isolates were found to be multi-drug resistant (resistant to 3 or more antibiotics belonging to different classes). The other sixty isolates were all resistant to at least one antibiotic with 52% being multidrug-resistant. These isolates exhibited resistance to ampicillin (37%), amoxicillin + clavulanic acid (92%), cefepime (12%), cefotaxime (25%), cephalexin (58%), cefixime (18%), doripenem (8%), meropenem (15%), imipenem (2%), gentamicin (5%), streptomycin (17%), tetracycline (35%), ciprofloxacin (3%), norfloxacin (3%), trimethoprim-sulfamethoxazole (15%), and chloramphenicol (3%).

The spread of antibiotic resistance in food systems is a critical problem because it threatens public health and the implementation of sustainable development goals (SDGs). Prompt actions are required on the national level to control the use of antimicrobials in all sectors in Lebanon. This urgent step might reduce the potentially devastating impacts of antibiotic resistance in Lebanon and contribute to delivering safe, healthy, and nutritious foods. These actions could be implemented by issuing laws to limit the excessive use of critical antibiotics in both agriculture and human medicine.

APPLICATION OF FORWARD OSMOSIS-MEMBRANE DISTILLATION CRYSTALLIZATION (FO-MDCr) HYBRID PROCESS FOR NEAR ZERO LIQUID DISCHARGE (ZLD) IN INDUSTRY PLANT

Mona Gulied,[1] **Sifani Zavahir,**[1] **Tasneem Elmakki,**[1] **Dong Suk Han**[1,2]

[1]*Center for Advanced Materials, Qatar University, PO Box 2713, Doha Qatar*
[2]*Department of Chemical Engineering, College of Engineering, Qatar University, Doha, Qatar*
* E-mail: mgulied@qu.edu.qa

To provide a minimum disposal of all types of water streams entering the Arabian Gulf Sea from Qatari industries, Qatar fertilizer company (QAFCO) is working to develop sustainable and economically effective methods to manage water streams generated within the QAFCO plant. QAFCO is one of the world's largest ammonia and urea producers, with a capacity of 12,900 metric tons per day, generating wastewater and brine solution from the Harbor-Bosch process and the multi-stage flash (MSF) desalination process, respectively. To protect the environment, zero liquid discharge (ZLD) is the best practice method to manage the waste streams of QAFCO facilities. Here, this study investigated the application of the forward osmosis (FO) and membrane distillation crystallization (MDCr) hybrid process for ZLD designed to minimize and concentrate wastewater to form crystal salts through a crystallizer. Both FO and MD are membrane-based processes. The FO process is driven osmotically across a hydrophilic microporous membrane, while the MD process is driven thermally through a hydrophobic microporous membrane. This research work aims to evaluate the performance of FO and direct contact membrane distillation (DCMD) processes in terms of water flux, % water recovery, % salt rejection, and fouling at various concentrations of feed solution (FS) and fixed concentration of draw solution (DS), FS temperature, and flow rates. First, the FO process was constructed to concentrate wastewater used as FS and utilize brine solution as DS. Then the DCMD process was then conducted to supersaturate the concentrated FS of the FO and feed it to a rotary evaporator to obtain crystallized solids. The obtained results of the FO process showed a decrease in water flux (12.48 to 8.25 LMH) and water recovery (22.45 to 14.85%) with increasing the salinity of the FS due to the low osmotic pressure gradient between FS and DS. Whereas the DCMD results exhibit a slight improvement of water flux (16 to 22 LMH) and water recovery (4.4 to 6.11%) at the high salinity of the FS, indicating that the temperature gradient between the feed side and permeate side is effective for high water recovery. The ongoing research work will optimize the operating conditions of individual processes to be combined to build a continuous FO-MDCr hybrid process to achieve QAFCO's ZLD strategy improvement.

ARTIFICIAL INTELLIGENCE BASED APPROACH TO DETECT BREAST CANCER

Mohammed R. AL-lami[1] , Falah S.[1] , Dheah S.[2]

[1]*Department of Chemistry / College of Science / Al-Mustansiriyah University / Baghdad-Iraq*

[2]*DNA Center for Research and Training / Al-Nahrain University / Baghdad-Iraq*

E-mail: mohammdry@gmail.com

Cancer is generally the deadliest diseases and might be the dangerous medical condition nowadays researched and reported in the literature in the global. Many institutions trying to find an early intervention to deal with such a complex and un predicted behaver of cells affected in the human body of people who are suffering from cancer. Breast cancer is the most and common type of cancer probably can be diagnosis in women. One of the challenge issue to obtain an efficient diagnosis to assist medical specialist in order to decide correctly on deferent cases.

One of the modern and an effective approach is artificial intelligence (AI) techniques to provide data analysis and modeling. In this work AI-based method was used to detect breast cancer.

Key Words; Breast cancer, Artificial intelligence, Detection

BIOSYNTHESISED TITANIUM DIOXIDE NANOPARTICLES FOR THE PHOTODEGRADATION OF METHYLENE BLUE (MB) DYE AND SULFISOXAZOLE (SSX) ANTIBIOTIC

Dineo A Bopape[1], Davide E Motaung[2] and Nomso C Hintsho-Mbita[1*]

[a]*Department of Chemistry, DSI/NRF Centre of Excellence in Strong Materials, University of Limpopo, PO Box X1106, Sovenga, 0727*

[b]*Department of Physics, University of the Free State, Bloemfontein, 9300, South Africa*

[*]*e-mail: dineobopape3@gmail.com*

There is a high increase in both man-made and naturally occurring pollutants contributing to water pollution. Methylene blue (MB) dye and the antibiotic sulfisoxazole (SSX) have both been found in natural water streams as toxic chemical contaminants. These pollutants have been treated using a variety of techniques, including chlorination, reverse osmosis, adsorption, and electrochemical destruction [1]. These methods have been shown to be either expensive, pollute the environment, or take a long time to complete the removal of contaminants [2]. One of the most highly suggested methods among the previously employed treatment methods is photocatalytic degradation. Existing photocatalyst synthesis methods, including sol-gel, polymerisation, hydrothermal, and solvothermal, depend on hazardous reagents as reducing and stabilizing agents [2]. Thus, utilizing *C. benghalensis* plant extract, in a simple, eco-friendly and cost-effective method for synthesising titanium dioxide (TiO_2) nanoparticles is presented in this study. Preliminary data showed that the 30 g *C. benghalensis*-mediated TiO_2 produced spherical materials with the smallest particle size and largest surface area of 50-200 nm and 174.6 ± 1.35 m^2/g, respectively. Upon degradating MB and SSX with the 30 g *C. benghalensis*-mediated TiO_2, a 68 % and 94 % degradation efficiency, respectively was noted. The OH species were responsible for the degradation and the materials could be reused at least two times.

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Blue Energy for sustainable industrial wastewater reclamation

Tasneem Elmakki,[1] **Fathima Sifani Zavahir,**[1] **Dong Suk Han**[1,2]

[1]Center for Advanced Materials, Qatar University, Doha Qatar

[2]Department of Chemical Engineering, Qatar University, Doha Qatar

E-mail: tasneem.sayedahmed@qu.edu.qa

Today's ever-growing advances in technology and process are on the brink of a massive increase in energy demand. Thus, the need for sustainable and decarbonized energy sources has become a primary goal worldwide. In this context, salinity gradient energy (blue energy) emerges as a promising sustainable and green energy source with the potential to lessen the need for those fuel-based sources. A prosperous technology in this blue energy field is reverse electrodialysis (RED). RED is a membrane-based electrochemical system that utilizes ion exchange membranes and electrodes to harvest the ionic charges from saline streams and convert them into viable electrical energy. RED membrane technology, which is thriving due to its ease of use, compactness, and portability, can serve as an energy-intensity reducer when integrated with other energy-demanding industrial processes such as reverse osmosis (RO), membrane distillation (MD), capacitive deionization (CDI), forward osmosis (FO), and various electrochemical systems. This study investigated the effect of concentrate and dilute stream concentrations, compositions, and flow velocities variation on power generation, and resulted in the highest gross power density attainment ($P_{d,\ net}$ = 2.17 W/m^2) when a low concentration (LC) solution of 0.015 M $(NH_4)_2SO_4$ (Simulated wastewater) was passed against a high concentration (HC) solution of 1 M NaCl (Simulated SWRO brine) at a flow velocity of 1.18 m/s. Additionally, the effect of flow mode alteration and extent of external load application was also examined and gave the most consistent energy acquisition attributes when single-pass mode with 10 Ω external loads where implemented.

CADMIUM COMPLEXES OF 1-SUBSTITUTED BENZOTRIAZOLE LIGANDS: STRUCTURAL AND PHOTOPHYSICAL PROPERTIES

Houda Al Sharji,[1] **Muna Al Mandhary**[1]

[1]*Department of Chemistry, Sultan Qaboos University, Muscat, Sultanate of Oman*

E-mail: s88517@student.squ.edu.om

Coordination polymers of metal ions have attracted attention for their optical, electronic, and magnetic properties [1]. Two imine type (N^N) bidentate ligands **(L1 & L2)** based on 1-substituted benzotriazole subunits linked with quinolone and quinoxaline were synthesized. The ligands were characterized by analytical and multi-spectroscopic techniques. Polymeric molecular cadmium complexes of the ligands, $[\mathrm{Cd}(\mathbf{L1})_2(\mu\text{-SCN})_2]_n$ **(1)** and $[\mathrm{Cd}(\mathbf{L2})(\mathrm{CH_3OH})(\mu\text{-SCN})_2]_n$ **(2)** were synthesized and characterized by several physical techniques, including single-crystal X-ray crystallography **(Fig. 1)**. The complexes have slightly distorted octahedral Cd centers with complex **1** having $\mathrm{CdN_4S_2}$ chromophore furnished by two benzotriazolyl N atoms of *trans*-oriented **L1** ligands and two S atoms and two N atoms of μ-1,3-bridging thiocyanate anions and complex **2** having a $\mathrm{CdN_3S_2O}$ chromophore furnished by one N atom of **L2** benzotriazolyl ring, two N atoms and two S atoms of μ-1,3-bridging thiocyanate anions, and one O atom of a $\mathrm{CH_3OH}$ molecule. Adjacent cadmium centers are bridged by a pair of μ-1,3-SCN anions to form 1D linear chain coordination polymers. The polymer chains of Cd complexes are linked to form 2D sheets by H-bonding interactions. The conformation of the metallacycles in both complexes are markedly different.

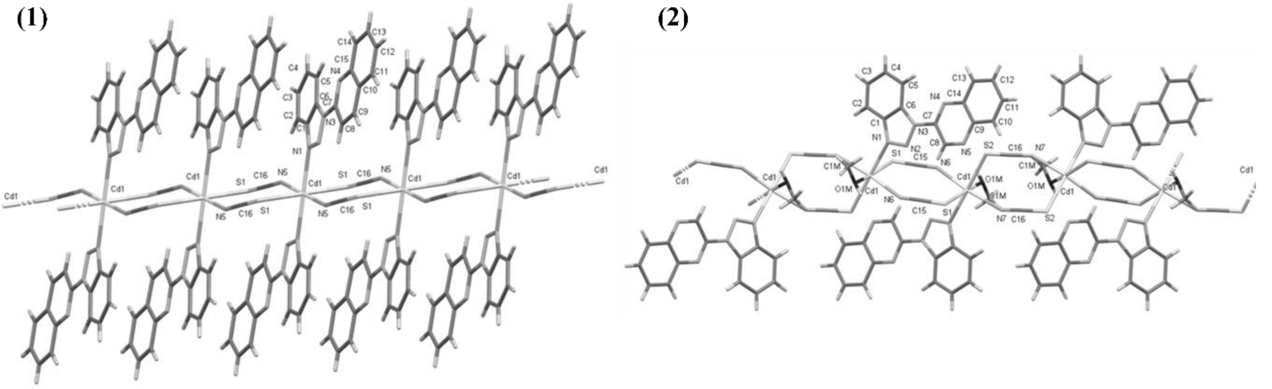

Fig. 1: Fragments of the polymer chains of $[\mathrm{Cd}(\mathbf{L1})_2(\mu\text{-SCN})_2]_n$ **(1)** and $[\mathrm{Cd}(\mathbf{L2})(\mathrm{CH_3OH})(\mu\text{-SCN})_2]_n$ **(2)**

UV-visible spectra of both complexes in solution exhibit only intra-ligand absorption bands. Solid-state emission spectra exhibit broad violet emission bands centered at 384 and 398 nm respectively when photoexcited at 330 nm. The emission bands of the complexes are blue-shifted relative to their corresponding uncoordinated ligands and their emission intensity are significantly enhanced, presumably due to increased conformational rigidity of the ligands upon coordination and reduction of energy loss by radiationless deactivation pathways. The onset decomposition temperature of complexes **1** (261 ℃) and **2** (258 ℃), determined by thermogravimetric analysis (TGA) show that they have high thermal stability, suitable for potential application as emitters in OLED devices.

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CALCIUM PHOSPHATE NANOPARTICLES: IMPROVED MECHANICAL PROPERTIES, FORMALDEHYDE-FREE AND HALOGEN-FREE FLAME RETARDANCY ON COTTON FABRIC

Laila Sadallah[1], Aziz Bentis[1,2], Aicha Boukhriss[2], Sanaa Majid[3] and Said Gmouh[1]

[1]Laboratory of engineering and materials, Hassan II University of Casablanca, Casablanca, Morocco.
[2]Laboratory on textile materials, Higher School of Textile and Clothing Industries, Casablanca, Morocco.
[3]Materials Engineering Laboratory for Environment and Recycling, Hassan II University of Casablanca, Casablanca, Morocco.
E-mail: l.sadallah2012@gmail.com

In this paper, we report on the application of calcium phosphate nanoparticles (CaP-NP) to cotton fabrics to improve their flame retardancy. A series of hybrid silica coatings were produced by the sol-gel technique using tetraethoxysilane (TEOS) as a precursor and calcium phosphate nanoparticles as a flame-retardant additive. The prepared sols were applied to the cotton fabric by the pad drying process. Characterization of the chemical composition and surface morphology of treated and untreated cotton fabrics was performed by Fourier Transform Infrared Spectroscopy (FT-IR) and Scanning Electron Microscopy (SEM), respectively. Thermogravimetric analysis (TGA) and Differential Scanning Calorimetry (DSC) were performed to identify thermal stability, pyrolysis properties, and amount of heat imparted, respectively. The flammability behaviour of functionalized tissues was evaluated by vertical flame tests. In addition, the impact of the CaP-NP-based coating on the tensile strength of the treated samples was evaluated using uniaxial tensile strength.

The results showed that treated cotton fabrics had excellent thermal stability and proved to have better mechanical properties than untreated cotton fabrics. These new halogen-free and formaldehyde-free hybrid coatings are simple, fast, effective, economical, and contribute to flame-spread retardance in the production of cotton fabrics with flame-retardant properties.

CARBON DOTs-MODIFIED PAPER-BASED CHEMILUMINESCENCE DEVICE FOR RAPID DETERMINATION OF MERCURY (II) IN COSMETICS

Iman Al Yahyai[١], Haider A.J. Al-Lawati[١], Javad Hassanzadeh[١]

[١] *Department of Chemistry, College of Science, Sultan Qaboos University, Box ٣٦, Al-Khod ١٢٣, Oman*

E-mail: iman.alyahyai@gmail.com

E-mail: haiderl@squ.edu.om

E-mail: javadhassanzadeh٦٣@gmail.com

Herein, a simple and portable paper-based analytical device (PAD) based on the inherent capability of carbon quantum dots (CQDs) to serve as a great emitter for the bis(٢،٤،٦-trichlorophenyl) oxalate (TCPO)-hydrogen peroxide (H_2O_2) chemiluminescence (CL) reaction is introduced for the detection of harmful mercury ions (Hg^{2+}). The energy is transferred from the unstable reaction intermediate (١,٢-dioxetanedione) to CQDs, as acceptors, and an intensive orange-red CL emission is generated at about ٦٠٠ nm, which is equal to the fluorescence emission wavelength of CQDs. The analytical applicability of this system was examined for the determination of Hg^{2+}. It was observed that Hg^{2+} could significantly quench the produced emission, which can be attributed to the formation of a stable and non-luminescent Hg^{2+}-CQDs complex. Accordingly, a simple and rapid PAD was established for monitoring Hg^{2+}, with a limit of detection (LOD) of ٠،٠٤ µg mL$^{-١}$. No interfering effect on the signal was found from other examined cations, indicating the acceptable specificity of the method. The designed assay was appropriately utilized to detect the Hg^{2+} in cosmetic samples with high efficiency. It is characterized by its low-cost, easy-to-use, facile but, accurate, and high selective for the detection of Hg^{2+} ions. Besides, the portability of this probe makes it suitable for on-site screening purposes. Compared with other works that used a similar CL system, the PAD-CL system reported in this paper shows a fantastic advantage in lowering the consumption of organic solvents (١٠ µL/ experiment), where all reagents except TCPO could be prepared in water without any problem.

Carcinogenic and Neurotoxic Risks of Dietary Acrylamide Consumed Through Cereals Among the Lebanese Population

Marlon Freiha, Areej Merhi, Robin Taleb

Department of Natural Sciences, School of Arts and Sciences, Lebanese American University, Byblos, Lebanon. Correspondence to robin.taleb@lau.edu.lb

The present study aims to determine the carcinogenic and neurotoxic risks associated with the consumption of acrylamide from cereal products. Acrylamide was extracted from cereal products, according to the method proposed by Biedermann, and analyzed on a UPLC-MS/MS Spectrometer. The results reveal that oat-based and mixed cereals contain the highest amount of acrylamide among cereal products with levels as high as 271 and 348 μg/kg, respectively. Children were shown to exhibit both carcinogenic and neurotoxic risks regardless of the type of cereal product consumed. For adults above 50 years of age, only consumers of oat-based cereal products seem to exhibit carcinogenic and neurotoxic risks. To avoid a carcinogenic and neurotoxic risk among the Lebanese population, we propose that the WHO/FAO set the maximum tolerable concentration for acrylamide in cereal products at 94.8 μg/kg product, a value which is 3-folds lower than the average acrylamide levels found in this study. Alternatively, and unreasonably, the average Lebanese population and children among the Lebanese population may choose to minimize cereal consumption by 1.7- and 7.2-folds respectively, should they want to avoid a health hazard as a result of acrylamide intake. All in all, the cereal product industry should respond by optimizing their production process in a way to reduce their acrylamide levels.

CATION-EXCHANGE RESINS FOR INDUSTRIAL WASTE WATER TREATMENT

Pulatov Kh.L., Aripdjanov O.Yu., Usmanova A.B.

Tashkent chemical-technological institute, Uzbekistan

oybek_396@mail.ru

ABSTRACT

There were obtained new cation-exchange resins by sulfonation and phosphorylation of styrene-furfural polymer. The value of the static exchange capacity for calcium, magnesium, copper, nickel, and cobalt ions was calculated for ion exchanger samples in contact with a solution of calcium, copper, nickel, and cobalt salt and a model solution for seven days. The conditions for the phosphorylation of this polymer were selected from the experiments accumulated in relation to the phosphorylation reactions of low- and high-molecular compounds. The resulting polymer had an exchange capacity for a 0.1N NaOH solution – 5,5-5,6 mEq/g and contained 16,5% phosphorus. Based on the studies carried out, the optimal conditions for the synthesis of the styrene-furfural polymer are assumed to be: the reaction temperature is 90°C, the concentration of the $ZnCl_2$ catalyst is 0.07 mol per mole of furfural, and the molar ratio of styrene to furfural is 1:1. The interaction of the cation exchanger in Na- and H-forms with solutions of salts of copper sulfate, nickel, cobalt, sodium chloride, calcium and uranyl nitrate was studied. In order to elucidate the mechanism of sorption of the cations of these metals, were taken the IR-spectra of the cation exchanger in the H and Na form, saturated with copper ions. According to the literature data, the vibration frequencies for phosphoric acid groups are in the range of 700-2560 cm^{-1}. In the spectrum of the cation exchanger in the H-form, bands are observed at 1150 cm^{-1}, corresponding to stretching vibrations of the phosphorus-oxygen bond. The absorption band at 1150 cm^{-1} does not disappear in the spectrum of the cation exchanger in the Na-form. The tested cation exchanger contains phosphoric acid groups differing in their acidic properties pK_1=2,8; pK_2=7,5. The less dissociated phosphoric acid groups, the stronger hydrogen bond forms phosphoryl oxygen with OH groups. Therefore, it can be expected that as the cation exchanger is saturated with sodium, the maximum of the band corresponding to the phosphorus-oxygen bond vibrations will slightly shift to longer wavelengths as a result of the destruction of the weaker hydrogen bond.

Key words: sorption, styrene, furfural, phosphorylation, cation exchange resin, ion exchange, thermal and chemical resistance, static exchange capacity, dynamic exchange capacity, mechanical strength.

CERAMIC COATED $LiNi_{0.5}Mn_{1.5}O_4$ MICROSPHERES WRAPPED IN GRAPHENE AS CATHODE MATERIALS FOR HIGH-VOLTAGE LITHIUM-ION BATTERIES

Zawar Qureshi,[1] Hanan Abdurehman Tariq,[2] Hiba Mohammed Hafiz,[1] Siham AlQaradawi,[3] Abdul Shakoor,[2] Ramazan Kahraman.[1]

[1]Department of Chemical Engineering, Qatar University, Doha, Qatar

[2]Center of Advanced Material, Qatar University, Doha, Qatar

[3]Department of Chemistry , Qatar University, Doha, Qatar

E-mail: shakoor@qu.edu.qa

Due to its high working voltage, low cost, and environmental friendliness, cobalt-free $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) has sparked considerable interest as a cathode material for lithium-ion batteries. LNMO cathodes, however, currently exhibit capacity degradation on cycling, severely limiting their commercial adaptability. Hence, microwave-assisted chemical co-precipitation was used to synthesize secondary spherical particles, containing primary nanoparticles of LNMO, that were subsequently coated with CeO_2 (LNMO-Ce) and wrapped in graphene (LNMO-Ce-GO). The ceria coating, together with the graphene wrapping, prevents undesired phases from developing and affecting the shape of the LNMO microspheres, according to structural studies. LNMO-Ce-GO has a discharge capacity of 131 $mAhg^{-1}$ at the 0.1C rate and a capacity retention of 98.6 percent after 100 cycles, compared to LNMO-Ce and bare LNMO samples, which exhibit capacities of 92 percent and 81 percent, respectively. The ceria coating aids in the suppression of unfavorable reactions at the cathode-electrolyte interface as well as the reduction of Mn^{3+} dissolution owing to the Jahn-Teller effect, hence boosting cell cyclability. The graphene matrix decreases material aggregation and creates conductive channels, which improves the electrochemical performance of the LNMO cathode dramatically. This novel material design technique may be easily applied to various types of lithium-ion battery cathode materials in order to improve their electrochemical performance.

CHARACTERIZATION AND APPLICATION OF NANOCOLLOIDAL Mn(IV) IN A CHEMILUMINESCNEC SYSTEM USING NANODROPLET MICROFLUIDICS PLATFORM

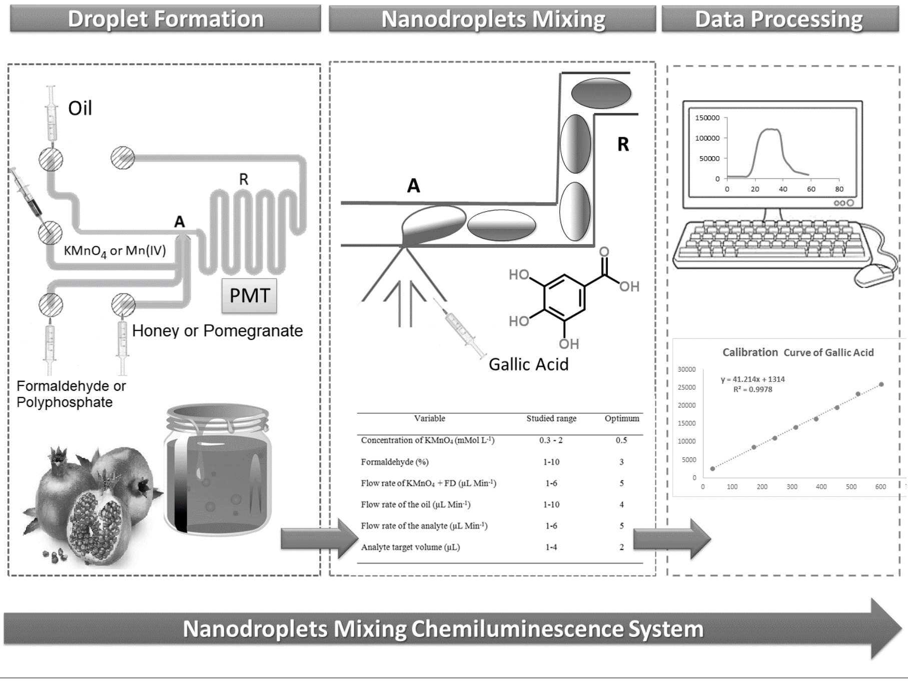
Baqia Al-Mughairy[1], Haider Al Lawati[2], and FakhrEldin O. Suliman[2]

[1]*Ministry of Education, Oman*
[2]*Department of Chemistry, College of Science, Sultan Qaboos University, Muscat, Oman*
E-mail: baqiah@hotmail.com

An extensive investigation has been carried out to test the nanocolloidal manganese (IV) chemiluminescence (CL) system and to utilize it for the determination of total phenolic content (TPC) in fruit juices. Initially, a detailed characterization of the produced nanocolloidal Mn(IV) was conducted including oxidation state, elemental analysis, size, shape and morphology. The electrochemical studies confirmed the oxidation state of Mn (IV), and the elemental analysis confirmed the formation of MnO_2. The size of the spherical nanocolloidal Mn (IV) was found to be approximately 5 ± 1 nm. Using these nanocolloidals, a new nanodroplet microfluidics chip was used to develop a CL method for the determination of the TPC in fruit juices. In comparison to the published work on the determination of TPC in food samples using nanocolloidal Mn(IV), the reduction in the flow rates of the proposed setup is 650- fold due to the novel chip design.

The novel chip consists of three main zones; a serpentine mixing zone, a CL nanodroplet reaction zone and a serpentine detection zone. These three zones were kept very close to each other such that the total area is less than 1.8 cm^2. This small area enabled fast and robust analysis despite the low flow rates utilized here.

The study was then extended to investigate 18 of the phenolic compounds that are commonly found in food samples. The limits of detection (LOD) obtained were between 1.3 ng mL^{-1} for gallic acid and 16.5 ng mL^{-1} for rutin. The proposed method is characterized by its excellent repeatability and reproducibility (0.4% and 4% respectively using gallic acid solution of 1000 ng mL^{-1}). The sensitivity and the selectivity of the nanocolloidal Mn(IV) CL toward phenolic compounds were compared with those obtained by the acidic $KMnO_4$ – formaldehyde CL system. Finally, the method was applied successfully to the determination of the TPC in pomegranate juice[1].



Variable	Studied range	Optimum
Concentration of $KMnO_4$ (mMol L^{-1})	0.3 - 2	0.5
Formaldehyde (%)	1-10	3
Flow rate of $KMnO_4$ + FD (µL Min^{-1})	1-6	5
Flow rate of the oil (µL Min^{-1})	1-10	4
Flow rate of the analyte (µL Min^{-1})	1-6	5
Analyte target volume (µL)	1-4	2

CHEMICAL REACTION ENGINEERING FOR THE DIRECT SYNTHESIS OF ORGANIC CARBONATES FROM CARBON DIOXIDE

Gasim Ibrahim,[1,2,3] Hanif A. Choudhury,[1, 3] Mohamed S. Challiwala,[1, 3] Dharmesh Kumar,[4] P. Sunifar,[4] Nimir O. Elbashir[1,3]
[1]*Chemical Engineering and Petroleum Engineering Program, Texas A&M University at Qatar, Doha, Qatar*
[2]*Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, USA*
[3]*TEES Gas & Fuels Research Center, College Station, USA*
[4]*Qatar Shell Research and Technology Center, Qatar Science and Technology Park, Doha, Qatar*
email: nelbashir@tamu.edu

A rapid increase in global carbon dioxide (CO_2) emissions has contributed to change in climatic conditions. Over the years significant scientific efforts have been made to identify viable solutions to address this global challenge. One approach to reduce CO_2 emission into the atmosphere is the chemical pathway, in which CO_2 molecules are chemically converted to sustainable products. However, CO_2 is a chemically stable molecule and requires significant amounts of energy to activate it. A common means of facilitating CO_2 reactions is via catalysis wherein the CO_2 molecules are adsorbed on the surface of the catalyst and interact with other precursors to then form products. One of the challenging aspect in CO_2 reactions is low conversion due to thermodynamic constraints even in presence of catalysts – example in conversion of CO_2 to Organic Carbonates.

In this presentation, we will highlight our efforts in developing a sustainable process for the direct synthesis of dimethyl carbonate (DMC) which involves reacting methanol and CO_2 to produce DMC and water. Catalysts with oxygen storage capabilities such as CeO, ZrO and mixed metal oxides of ceria and zirconia are reported to be active and selective towards direct DMC synthesis. We synthesized catalysts using xero-gel method and co-precipitation techniques, and the performance of these catalysts was evaluated in a slurry reactor under batch condition of 30 bar pressure and 110 °C temperature. The catalysts exhibited significantly different conversions towards DMC, but all below 1% conversion – in line with our thermodynamic assessment. Furthermore, life cycle assessment study show that the process is CO_2 neutral and negative only when the reaction has a conversion below 4% under low pressure conditions. Thus to approach this target, we attempt to shift the equilibrium conversion by utilizing methods for in-situ removal of water, which shifts the equilibrium in favor of the forward reaction. In our test with physical adsorbents such as activated carbon, Dowex, and 5A molecular sieves did not show any improvement in the methanol conversion towards DMC. However, addition of 2-CP as a water scavenger even at a low-pressure reaction condition of 5 bar showed significant improvement in methanol conversion towards DMC. An optimization of 2-CP system for low pressure condition of 5 bar is underway to approach the conversion needed to make the direct synthesis of DMC viable reaction pathways for CO_2 sequestration.

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Chemistry to resolve a worldwide pandemic, COVID-19.

Juliana C. Ferreira[1], Samar Fadl[1], Wael M. Rabeh[1*]

[1]Science Division, New York University Abu Dhabi, PO Box 129188, Abu Dhabi, UAE

E-mail: Wael.Rabeh@nyu.edu

Coronaviruses cause acute infections of the upper and lower respiratory tracts with mild to lethal symptoms. One of the most prominent coronaviruses is SARS-CoV-2, the virus responsible for coronavirus disease 2019 (COVID-19), which has caused millions of infections and deaths worldwide as well as major social and economic unrest. SARS-CoV-2 is one of the largest positive-sense, single-stranded RNA viruses and belongs to the genus Betacoronavirus, which also includes severe acute respiratory syndrome coronavirus (SARS-CoV) and Middle East respiratory syndrome coronavirus (MERS-CoV). The main protease of SARS-CoV-2, 3C-like protease (3CLpro), is one of two proteases responsible for processing two polypeptides to liberate 16 non-structural proteins (nsps). The nsps are important for replication, transcription, and virus recombination during infection. Inhibiting the proteases will block the release of the nsps and the progression of COVID-19, making 3CLpro an attractive target for the design of broad-spectrum antivirals against COVID-19.

In my lab, we characterized the functional and chemical properties of 3CLpro protease with optimum conditions for the high throughput screening of small molecules to identify existing FDA drugs as potential therapeutics for COVID-19 or new chemical compounds to be developed for the same. The various coronaviruses have identical structural folds of 3CLpro that forms a homodimer in which the two monomers are arranged perpendicular to each other. Studies of 3CLpro from different coronaviruses has suggested the dimer to be the catalytically active form, making the dimerization interface a target for antiviral development. Guided by structural analysis, single amino acid substitutions were introduced at nine residues at three key sites of the dimer interface to assess their impact on dimerization and activity. Four residues in two sites have been identify to be important for the activity of the protease, These results provide insights on two allosteric sites, R4/E290 and S10/E14, that may promote the design of antiviral compounds that target the dimer interface rather than the active site of SARS-CoV-2 3CLpro for higher efficacy and specificity.

CO-FEEDING OF MINERALS-RICH BIOCHAR ON THE PYROLYSIS PRODUCTS FROM FOOD WASTE

Ayman Mohamedelkhair[1], Yassir Makkawi[1], Yehya El Sayed [2]

[1] Bioenergy and Solar Conversion Research Group (BSCRG), College of Engineering, American University of Sharjah, P.O. Box 26666, Sharjah, United Arab Emirates (UAE).

[2] Department of Biology, Chemistry and Environmental Science, American University of Sharjah, P.O. Box 26666, Sharjah, United Arab Emirates (UAE).

Food waste (FW) is one of the most abundant unrecycled products in our contemporary ecosystem. This poses waste management issues and negative environmental impacts. In this study, experiments on the pyrolysis of co-feeding of food waste with biochar-rich minerals were conducted at 550 °C. The results show significant differences in the gas and bio-oil characteristics in the case of co-feeding, mainly due to the catalytic effect of biochar minerals. In the case of co-feeding, the CH_4 and H_2 fractions in the gas are 50% higher, respectively, the aqueous phase fraction in the pyrolysis liquid is 165% higher, while the bio-oil yield is 62% lower. These results suggests that the presence of mineral-rich biochar in the feedstock enhances catalytic cracking of the pyrolysis gas and increases the production of reaction water. However, quantitatively, there is limited impact on the overall product percentage distribution. The outcome of this study is hoped to pave the way for future development and optimization of food waste pyrolysis, while contributing to the global effort on reducing waste going into landfills.

Keywords: Pyrolysis, Food waste, Biomass co-feeding, waste minimization

COMBINING FUNCTIONALISED NANOPARTICLES AND SERS FOR THE DETECTION OF miRNA BIOMARKERS RELATED TO A TYPE 2 DIABETES

Laila Al-Maqbali,[1] Karen Faulds,[2] Duncan Graham[2]

[1]*Department of Chemistry, Sultan Qaboos University, Muscat, Sultanate of Oman*

[2]*Centre for Molecular Nanometrology, Department of Pure and Applied Chemistry,*
University of Strathclyde, Technology and Innovation Centre, 99 George Street,
Glasgow, G1 1RD

E-mail: lailak@squ.edu.om

MicroRNAs (miRNAs) are short non-coding RNA with a length of 18 to 24 nucleotides found in plants, animals, and some viruses. They modulate protein expression by binding to complementary sequences of messenger RNA (mRNA) and are likely to be involved in most biological process by affecting gene regulation. They were discovered in the 1990s, however they were not recognised as a class of biological regulators until 2000. Since then, they have attracted a lot of attention for their potential use in the treatment and prevention of many diseases like cancer, cardiovascular diseases and type 2 diabetes.

Many methods can be used for miRNA biomarkers detection but Surface Enhanced Raman Scattering (SERS) is considered to be fast, highly sensitive and an extremely effective technique for miRNA detection when used with bio-functionalised metallic nanoparticles. The development of an assay for miRNA detection using SERS is of great importance, as it will open an avenue for treating many diseases through miRNA biomarkers. However, RNA is generally known for its chemical instability unlike DNA, which is the most challenging problem, associated with RNA. The assay designed for the miRNA detection should overcome this problem and develop a stable method for the detection of miRNA biomarkers in solution.

Recent studies have shown a correlation between circulating miRNA and type 2 diabetes. Moreover, miRNA profiling has been proven to be deregulated in patients with type 2 diabetes. So, the development of an assay to detect miRNA biomarkers would allow for early detection of type 2 diabetes as this disease have along asymptomatic period and potentially reduce the numbers of people with undiagnosed diabetes who could develop devastating and costly complications like strokes, blindness, nerve damage, foot diseases and heart diseases.

DNA nanoparticle conjugates were synthesised and used to detect specific miRNA sequences related to type 2 diabetes. Hybridisation of miRNA target with the DNA conjugates was followed by extinction spectroscopy and showed a red shift indicating a specific hybridisation had taken a place. Adding a dye SERS tag allowed hybridisation to be followed by SERS and demonstrate a change in intensity following miRNA hybridisation. This shows a great promise for the use of DNA nanoparticle conjugates and SERS for the detection of miRNA biomarkers related to type 2 diabetes such as miRNA29a and miRNA126.

Computational Design of Organo-Chalcogen Fluorescence Sensors

Reem R. Habash[1], Akef T. Afaneh[1] and Mansour H. Almatarneh[2]

[1]Department of Chemistry, Faculty of Science, Al-Balqa Applied University, P. O. Box 206,
postal code 19117, Al-Salt, Jordan
[2]Department of Chemistry, University of Jordan, Amman 11942, Jordan
E-mail: reem-habash@hotmail.com, umafaneh@bau.edu.jo, m.almatarneh@ju.edu.jo

Abstract

This work aims to establish and validate a computational protocol to design fluorescence sensors with reasonable understanding. The structures and the vibrational frequencies of the tripod type sensors (S, Se and Te) have been computed using the B3LYP, PBE and M06-2x with different basis sets (6-31+G(d,p), 6-311+G(d,2p) and def2-TZVP). The results of GIAO‒NMR calculations are compared with the experimental data. The singlet and triplet excited‒states of the corresponding sensors are fully optimized using time‒dependent density functional theory (TDDFT). The behaviors of the molecular fluorescent probes will be examined through the complexation with heavy metal (II) ions (Cd^{2+} and Hg^{2+}) [1,2].

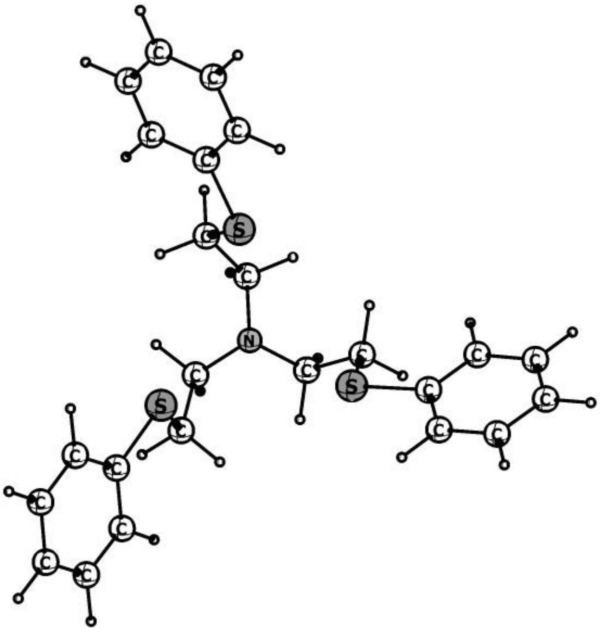

Figure: A tripodal system‒sulfur fluorescence sensor.

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COMPUTATIONAL FLUID DYNAMIC (CFD) MODELING OF DATE PALM WASTE STEAM GASIFICATION IN A CIRCULATING FLUIDIZED BED REACTOR

Feras Kordi [1], **Yassir Makkawi** [1], **Yehya El Sayed** [2]

[1] *Bioenergy and Solar Conversion Research Group (BSCRG), College of Engineering, American University of Sharjah, P.O. Box 26666, Sharjah, United Arab Emirates (UAE).*

[2] *Department of Biology, Chemistry and Environmental Science, American University of Sharjah, P.O. Box 26666, Sharjah, United Arab Emirates (UAE).*

B00059055@alumni.aus.edu

Abstract

This study presents a computational model and predictions of date palm waste gasification in a Circulating Fluidized Bed Reactor (CFB). Date palm waste is an abundant biomass resource in the Gulf and MENA region. For example, the UAE produces 500,000 tons of date palm waste annually, out of which only 50,000 is recycled, while the rest goes into landfills. This waste can be utilized as a key feedstock for future development of bioenergy in these regions. A state-of-the-art computational model has been developed to predict the complex hydrodynamic and thermochemical behavior of an industrial-scale CFB reactor (processing capacity of 1300 tons of biomass per day). Preliminary results suggests that date palm waste steam gasification is of high potential to produce hydrogen-rich gas (~50 mass% H_2), which is greatly enhanced by the thermal cracking of tar, homogeneous methane steam reforming, and water-gas shift reactions. The proposed process can be utilized for scale-up or scale-down studies, and the fully developed model will be flexible to changes in feedstock characteristics. Further enhancement of the gas quality has been achieved by catalysts effect induced by the injection of mineral-rich biochar and calcium oxide (burnt lime) to the reactor. The latter, calcium oxide has been found to be highly effective in the capturing of carbon dioxide, hence considerably helpful in increasing the calorific value of the produced gas and in reducing GHG emissions. The proposed process is expected to play a major role in energy diversity in the Gulf and MENA regions as well minimizing waste going into landfills.

COST-EFFECTIVE SYNTHESIS AND APPLICATION OF CHITOSAN MODIFIED *ACACIA NILOTICA* BIO-COMPOSITE FOR REAL INDUSTRIAL WASTEWATER TREATMENT AND SIGNIFICANCE OF RSM FOR PARAMETRIC OPTIMIZATION

Muzammil Hussain[1], Shahzad Ali Shahid Chatha[1], Abdullah Ijaz Hussain[1], Kiran Aftab[1], Tanvir Ahmad[2]

[1]Department of Chemistry, Government College University Faisalabad, Pakistan

[2]Department of Statistics, Government College University Faisalabad, Pakistan

Email: muzamilhayat78@gmail.com

Water pollution is a thoughtful environmental and life-threatening issue due to rapid industrial growth. Industrial wastewater treatment is a challenging process and the choice of material from the pool of available material and parametric optimization using statistical tools is scanty. In the present research work, the bio-composite was synthesized using biochar of *Acacia nilotica* and chitosan, for the parametric optimization the design of the experiment was investigated using response surface methodology (RSM) with central composite design three-factor at five levels. The analytical characterization was showing amorphous structure (X-ray diffraction), good stability (Thermogravimetric analysis), porous surface (Scanning electron microscope) of synthesized bio-composite, and $-NH_2$, -OH functional groups (Fourier transform Infrared spectroscopy) on composite playing significantly major role for adsorption of heavy metals. The variation in ANOVA with a $p\text{-value}<0.05$ indicates model fit for parametric optimization. Thus, obtained results were showing excellent removal percentage of metals (Pb 84.70%, Cr 68.67%, Ni 77.02%, and Cd 93.21%) at (pH 6, contact time 60 min, and adsorbent dose 0.5g) statistical proved optimized parametric conditions. It is very reasonable to conclude that the synthesized chitosan-modified biochar composite is a promising material for multi-metals contaminated real industrial wastewater treatment.

CRYSTAL ENGINEERING OF MULTICOMPONENT CRYSTALS: MATERIAL DISCOVERY VIA COMPUTATIONAL AND MECHANOCHEMICAL APPROACH

Zeinab M. Saeed[1], Tamador Alkhidir[1], Bhausaheb Dhokale[1], Abeer F. Shunnar[1], Eman Abujami[1], Runyararo M. Nyadzayo[1], Sharmarke Mohamed[1]

Department of Chemistry, Green Chemistry & Materials Modelling Laboratory, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates

Crystal engineering is an effective strategy to modify the solid-state properties of crystalline materials including their mechanical, optical, and solubility properties. Over the past three decades, there have been reliable advancements in the computational and experimental methods for guiding the discovery of new multicomponent crystalline materials (i.e. cocrystals, ionic cocrystals, salts, solvates, and eutectics) with desirable properties. Example of well-known guiding principles that support the formation of binary cocrystals are ΔpKa, use of Hansen solubility parameter (to guide miscibility of candidate molecular pair), selection of complementary heterosynthons, not to mention the use of computational tools such as state of art dispersion-corrected density functional theory (DFT-D) to support the selection of suitable coformers. In contrast, the crystal engineering of higher order ionic cocrystals-ICCs (comprising of >2 components) is not well established, thus, an extensive survey was conducted on a total of 94 ICCs crystal structures retrieved from Cambridge structural database (CSD) [1]. The ICCs molecular and crystal properties were determined using computational tools, and we suggested that targeting higher order ICC requires selection of molecules with comparable number of conformational degrees of freedom, and significantly different polar surface area (between acid-base pair). In addition, ICCs formation were favored when ΔpKa of acid-base were in the range of $-1 < \Delta pKa < 4$, which is the gray zone of salt-cocrystal continuum. DFT-D calculations manifested that ICCs formation is enegertically driven, with an average lattice stabilization energy of -5 kJ mol^{-1}.

Another area that remains unexplored and poorly understood is the crystal engineering of eutectics due to the lack of reliable computational and empirical tools in targeting their formation. We conducted mechanochemical synthesis of three polycyclic aromatic hydrocarbons (PAH)/conformer eutectic solid forms. This was done using an “anti-crystal engineering” design principle where synthon incompatibility and molecular shape mismatch was found to be an important driver in eutectic formation. Computational structure prediction calculations using DFT-D show that eutectic formation is not thermodynamically driven as none of the PAH-coformer combinations led to stable solid form relative to the stabilities of the original components, with an average interaction energy of 2.60 kJ mol^{-1} across the composite series. Using Monte-Carlo simulation, mixing energies of eutectic components and their binding modes were computed and lead to temperature-dependent interaction parameter which predicted the likelihood of formation of eutectic. Eutectic solid formulations are desirable vehicles for physicochemical property optimization for molecules lacking functional groups (cannot form directional hydrogen bonding such as PAH). This is indicated by the observation of significant melting point depressions for the PAH upon eutectic formation that are in the range 19–51 °C relative to the PAH. Moreover, equilibrium solubility measurements reveal that the eutectics lead to a ~ 2–5-fold enhancement in the PAH solubility [2].

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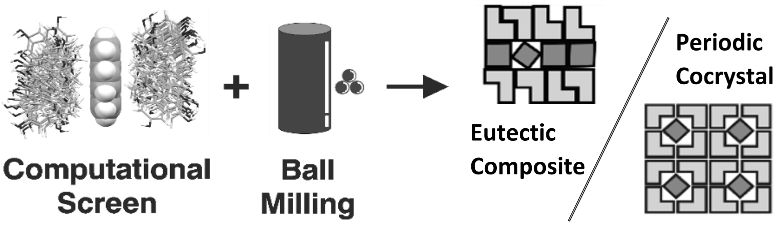

Deciphering the Therapeutical Potentials of Rosmarinic Acid

Fatima Naseraldine[1], Sally El Kantar[1], Ali Yassin[1], Louis Labaki[1,2], Sara Mitri[1], Alejandra Garcia-Maruniak[2], Elias Akoury[1]

[1] Department of Natural Sciences, School of Arts and Sciences, Lebanese American University, Beirut 1102-2801, Lebanon

[2] Santa Fe College Perry Center Emerging Technologies, 14180 NW 119 Terrace, Alachua, FL 32615, USA

Correspondence to elias.akoury@lau.edu.lb

Lemon balm is a herbal tea known for its therapeutic practice in soothing stomach cramps, indigestion and nausea. One of its chemical components is rosmarinic acid (RA), known for its antioxidant, anti-inflammatory antiviral, and anti-microbial activities. RA is known for its therapeutic potentials in cancer therapy, inflammatory diseases, and neuronal diseases such as the treatment of neurofibromatosis or prevention from Alzheimer's diseases (AD). RA has been also investigated against COVID-19. Despite efforts, the recovery and purification of rosmarinic acid from Lemon balm in high yields has not been entirely successful. Here, we report the aqueous extraction of rosmarinic acid from dried leaves of Lemon balm in high yields and decipher its structure by NMR spectroscopy. Using various physical-chemical techniques and biological assays, we then highlight the properties of RA in anti-aggregation inhibition, anti-cancer treatment, anti-bacterial activities, and antioxidant properties. The anti-aggregation potentials of RA against the formation of Tau filaments, one of the hallmarks of AD, was deciphered. We then demonstrate that RA causes a reduction of the mitochondrial reductase activity in tumor cells using cell viability and proliferation assays. We also investigate the antibacterial activity of RA, as a pure individual compound and its electrochemical properties by cyclic voltammetry. Our data demonstrates that RA is a prominent biologically active natural product and provides the most direct evidence for the therapeutic potentials for drug discovery in Alzheimer’s disease, cancer therapy and inflammatory diseases.

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Design of an anti-MUC1 monoclonal antibody via High Throughput Free Energy screening

Christopher Barnett[1], Kyllen Dilsook[1]

[1] Scientific Computing Research Unit and Department of Chemistry, University of Cape Town, Rondebosch, 7701, South Africa. Email: dlskyl001@myuct.ac.za

Source code: https://github.com/KyllenD/antibody-design

Cancer is one of the leading causes of death globally, accounting for 10 million deaths in 2020 with lung, stomach, colon, liver and breast cancers remaining the leading causes.[1] A hallmark common to these cancers is the altered sugar attachment or glycosylation of the MUC1 protein. In healthy cells, the MUC1 consists of long, branched sugars, whereas in cancer cells, these sugars are truncated.[2] This key difference makes MUC1 a viable target for antibody treatment.

The problem with cancer cells is that they are very similar to healthy cells. An effective antibody for detection and treatment of epithelial cancers should therefore be highly specific, recognizing the MUC1 peptide and the truncated sugar. My research will attempt to create this highly specific antibody making use of methods such as docking (PIPER), single state antibody design (Rosetta design), molecular mechanics (MM/GBSA), molecular dynamics (GROMACS) and GPU-accelerated Free Energy methods. Amino acid substitutions were introduced to the antibody structures obtained from the Protein Data Bank (PDB), using a combination of knowledge-based and physics-based energy functions. The effects of these substitutions on antigen-antibody binding were then characterized using free energy methods and further investigated using structural analytic methods.

This study will consider the Tn glycosylated MUC1 ligand as this truncated sugar variant is present in high concentrations in breast cancers.[3]

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DEVELOPMENT OF NANOEMULSION BY USING THE BIOGENIC SOURCE: AN IMPRESSIVE APPROACH TO OVERCOME THE CHALLENGES OF THE SURFACE QUALITY OF LOW CARBON METAL SHEETS AT AN INDUSTRIAL SCALE

Muhammad Ajmal[1], Syed Abid Ali[2], Hajira Tahir[1], Muhammad Raza Shah[2] and Muhammad Saad[1]

[1]*Department of Chemistry, University of Karachi, Karachi-75270, Pakistan*

[2] *Third world Center for Science and Technology, H.E.J. Research Institute of Chemistry, University of Karachi, Karachi-75270, Pakistan*

m.ajmal14@hotmail.com abid.ali@iccs.edu hajirat@uok.edu.pk raza.shah@iccs.edu saad@uok.edu.pk

Abstract

Oil-in-water emulsions are extensively used in the cold rolling process of metal processing industries. The basic theme of the reported research work is the simplistic and effective synthesis of the bio-based emulsion by modification of the titanium dioxide nanoparticles (TiO_2Nps). The experimental work was carried out in two temperature control phases. In the first phase, mustard oil was modified by the addition of Tergitol Np-7 surfactant, and TiO_2Nps. The method of sonication was adopted for the dispersion of TiO_2Nps in oil. In the second phase, the modified oil was utilized for the synthesis of emulsion under massive agitation. The characteristic results significantly reflect the stability and efficiency of bio-based nanoemulsion (BNE) like the Dynamic light scattering (DLS) show the less PDI 15.9%, and appropriate droplet size, 78.89nm these parameters are further collated with pH, conductivity, SEM, and ZP. The visual stability of BNE was monitored at different time scales and its impact on low carbon metal sheets was also investigated. Interestingly, it is observed that the newly developed BNE heightens the surface quality of metal sheets than any other conventional emulsions. Moreover, the synthesis by using the green source significantly opens up new avenues and would be an economic booster for metal processing industries.

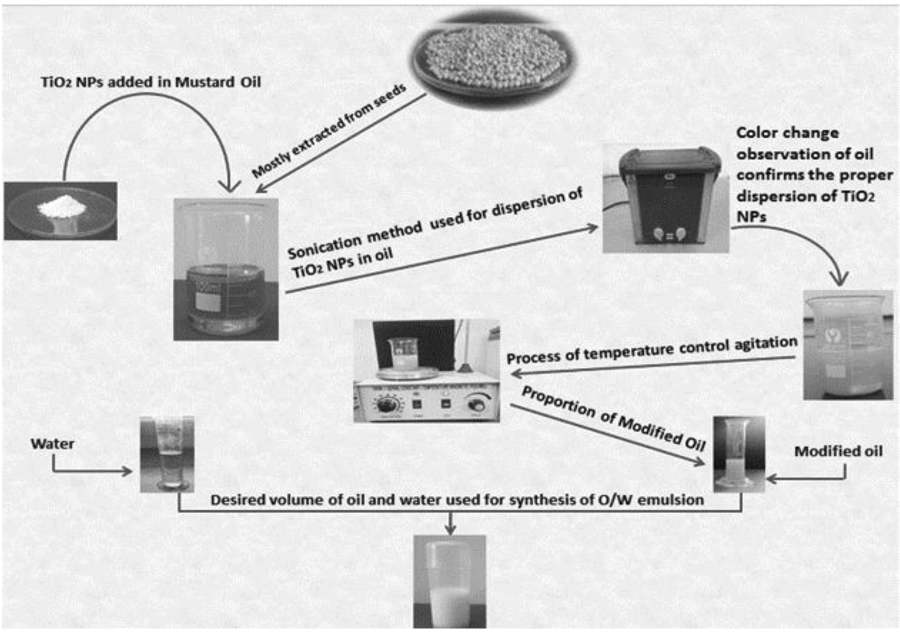


Fig 1: Schematic representation of the synthesis of oil-in-water emulsion

Did JUUL Alter the Content of Menthol Pods in Response to FDA Flavor Ban?

Amira Yassine,[1] Rachel El-Hage,[1,4] Ahmad El Hellani,[1,4] Rola Salman,[2,4] Soha Talih,[2,4]
Thomas Eissenberg,[3,4] Alan Shihadeh,[2,4] and Najat A. Saliba[1,4]

[1] *Chemistry Department, American University of Beirut, Beirut, Lebanon.*
[2] *Mechanical Engineering Department, American University of Beirut, Beirut, Lebanon.*
[3] *Psychology Department, Virginia Commonwealth University, Richmond, Virginia, USA.*
[4] *Center for the Study of Tobacco Products, Virginia Commonwealth University, Richmond, Virginia, USA.*
E-mail: ns30@aub.edu.lb.

JUUL captures a great share of the e-cigarette market in the US, and it is highly prevalent among youth. In response to the high popularity of JUUL and similar devices among youth, the US FDA issued a ban on the sales of all flavored cartridge/pod-based e-cigarettes in February 2020. This ban exempted tobacco and menthol-flavored pods. Subsequent studies showed that some users of the now-banned flavored JUUL pods (especially mint-flavored) switched to menthol-flavored JUUL pods with similar satisfaction. In this study, we sought to examine whether JUUL's liquid formulations changed in the years surrounding the flavor ban. We quantified menthol, nicotine, propylene glycol (PG), and vegetable glycerol (VG) in JUUL pods samples (Menthol, Classic Menthol, and Cool Mint) that were purchased in 2017, 2018, and 2020 (only menthol) to monitor differences before and after the ban. We also analyzed the samples to detect other cooling agents using a screening GC-MS headspace method. Our results showed that the PG/VG volume ratio was 27/63 in all pods. However, nicotine and menthol concentrations were significantly higher in the 2020 products than in the products from the prior years. Moreover, different profiles of cooling agents were detected in the tested pods. In conclusion, this study highlights that tobacco product manufacturers may increase product abuse liability in response to regulations intended to reduce it.

DIVERGENT ACTIVITY OF GRUBBS CATALYST: RING CLOSING METATHESIS AND OXACYCLOISOMERIZATION. OBTENTION OF CARBOBICYCLES AND FUSED BICYCLIC DIHYDROFURANS.

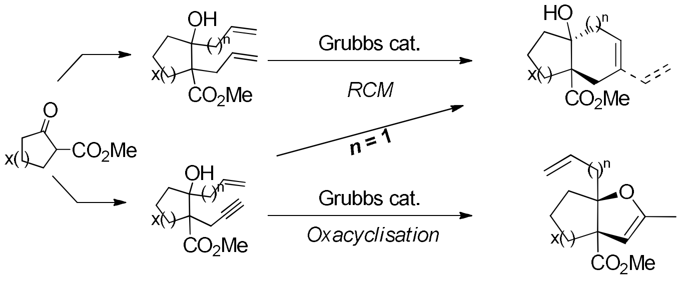
Assya Taleb,[1] Mokhtar Lahrech,[2] Salih Hacini,[1] Jérôme Thibonnet,[3] Jean-Luc Parrain[4]

[1]Laboratoire de Chimie Fine (L.C.F), University Oran1, BP-1524-Menouar,31000- Oran, Algeria
[2]Laboratoire de Chimie Organique et Subst.Nat (LCOSNa), University of Djelfa, Algeria
[3]Laboratoire SIMBA EA 7502, Dept Chimie, University of Tours, France
[4]Aix-Marseille University, CNRS, ISM2, Marseille, France
E-mail: s_hacini@hotmail.com ; hacini.salih@univ-oran1.dz

The development of highly active Grubbs-type ruthenium carbene complexes as catalysts of olefin metathesis has revolutionized organic synthesis. This reaction allows the synthesis of diverse cyclic and polycyclic compounds, from simple building blocks. [1]

This study focuses on a double result of reactions catalyzed by the first generation Grubbs catalyst: expected metathesis and a new example of non-metathetic reactions. Indeed, two divergent activities of the Grubbs catalyst are observed from different cycloalkanols, with the rapid construction of carbo-bicyclic systems by RCM of enene and enyne systems while bicyclic dihydrofurans are obtained by a catalytic oxycloisomerization reaction. [2]

Starting from simple cyclic 1,3-ketoesters, a three-steps sequence including allylation or propargylation, 1,2-addition reaction of functional Grignard reagent and alkylidene ruthenium catalysed cyclisation yields to carbobicycles and/or bicyclic dihydrofurans depending on the nature of the substituents of the enyne type reactants.



On the other hand, this reaction was extended to akynes having two alcohols functions providing polycyclic acetals with complete diastereoslectivities.

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EFFECT OF AN ELECTRIC FIELD ON THE POLYMORPHIC TRANSITION OF COBALT HYDROXIDE IN THE REACTION-DIFFUSION FRAMEWORK

Malak El Kaassamani, Manal Ammar and Mazen Al-Ghoul
Department of Chemistry, American University of Beirut, Beirut, Lebanon
E-mail: mazen.ghoul@aub.edu.lb

Crystalline cobalt hydroxide exists in two polymorphs, α and β[1], and possesses exceptional physical and chemical properties that make it an attractive constituent in heterogeneous catalysis, supercapacitors and various electronic and magnetic materials[2]. While the hydrotalcite-like blue α-$Co(OH)_2$ is expected to have a higher electrochemical activity than the pink brucite-like β-$Co(OH)_2$ due to its interlayer spacing and rich ion-exchange dynamics, they are difficult to synthesize because the α-phase is metastable and transforms rapidly to the β-form during synthesis or upon storage in strong alkaline media. Herein, we use the reaction-diffusion framework (RDF)[3] with imposed small-scale electric fields to control this polymorphic transformation. A direct electric field is applied using two circular electrodes with voltages ranging between 0.5 V and 1.65 V in a two-dimensional reactor at room temperature for a specific timeframe. The results indicate that the direction and strength of the electric field favor the gradual production of one polymorph over the other up to complete suppression of one of the polymorphs beyond a voltage threshold. When the central electrode is negative, α-$Co(OH)_2$ readily transforms into β-$Co(OH)_2$ in a short period, and the behavior is fully reversed with field reversal. SEM images confirm that the formation of α-$Co(OH)_2$ results in small nanoflakes, whereas β-$Co(OH)_2$ has a remarkably more significant hexagonal plate morphology with sharp edges, and that this transformation occurs according to a dynamic Ostwald ripening mechanism. In the second part of this work, we apply an alternating electric field that varies in time as a square wave. As a result, patterns of revert spaced precipitation bands of alternating polymorphs are induced. The banding pattern is controlled by the intensity and frequency of the electric field.

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EFFECT OF MODIFIED PARTICLES ON BARRIER PROPERTIES OF POLYOLEFIN COATINGS FOR CORROSION PROTECTION OF CARBON STEEL

Sehrish Habib[1,3], Muddasir Nawaz[1], Ramazan Kahraman[2,*], Elsadig Mahdi Ahmed[3], R. A. Shakoor[1,*]

[1]Center for Advanced Materials (CAM), Qatar University, 2713 Doha, Qatar.

[2]Department of Chemical Engineering, Qatar University, 2713 Doha, Qatar.

[3]Department of Mechanical and Industrial Engineering, Qatar University, 2713 Doha, Qatar.

Email: shakoor@qu.edu.qa

Corrosion results in considerable materials and equipment failure. According to one survey, about 1/4 to 1/3 of the total interruption in industries is due to detrimental effects of corrosion. A very effective route to protect metallic (and non-metallic) assets against corrosion is by the application of protective organic coatings. Protective coatings must ensure high barrier properties and mechanical strength. Polyolefin coatings have excellent mechanical properties and display very efficient polymer healing ability.

This work reports the corrosion inhibition performance of modified hybrid particles reinforced into polyolefin matrix. The cerium oxide coated zinc oxide hybrid particles (CeO2@ZnO) were synthesized via chemical precipitation process. The synthesized hybrid particles were then modified with benzotriazole (BTA, corrosion inhibitor). Transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR), Energy dispersive X-Ray spectroscopy (EDX), and X-ray photoelectron spectrometer (XPS) analysis techniques were employed to characterize synthesized and modified hybrid particles. The results demonstrated that ZnO possessed hexagonal morphology covered with spherical CeO_2 particles. FTIR analysis revealed the presence of characteristics peaks of the modified hybrid particles. UV-vis spectroscopic analysis confirmed the release of the inhibitor from hybrid particle which was pH and time dependent. The self-healing functioning of the modified polymeric coatings were evaluated through Electrochemical impedance spectroscopic analysis. The results revealed the prominent corrosion inhibition performance of modified coatings as compared to the blank polyolefin coatings which is attributed to the efficient release of the inhibitor from hybrid particles, making these coatings a promising solution for the protection of steel.

EFFECT OF MOLECULAR WEIGHT OF THE SILICONE RUBBER POLYMER MATRIX ON THE HIGH VOLTAGE INSULATION COATINGS

Fadi Z. Kamand, [1] Belal Saleh, [1] Safa Alkhalil, [2] Najlae Adnane, [2] Mohammad K. Hassan, [1] Leena Al-Sulaiti[1]

[1]*Center for Advanced Materials, Qatar University, P.O.Box 2713, Doha, Qatar*

[2]*Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University, P.O. Box 2713, Doha, Qatar*

Email: fadi.kamand@qu.edu.qa

Silicone rubber (SiR) coatings on porcelain or glass fiber core had been widely utilized for outdoor high voltage power transmission systems due to the high hydrophobicity, hydrophobicity self-recovery, low surface energy, and lightweight. Polydimethylsiloxanes (PDMS) based coatings are exposed to degradation under the effect of high voltage electrical stress and harsh environmental aging conditions such as ultraviolet (UV) exposure, high temperature and humidity levels, sand collisions, and accumulation of salts. In addition, industrial pollutants and ozone gas from the arcing and corona are also important parameters to be considered for the long time performance of the RTV coatings. Environmental degradation can promote loss of hydrophobicity, which results in an uncontrolled leakage current, arcing, and flashover. These factors can cause costly electrical power failure. Inspired by this, herein, a novel study was performed to investigate the impact of molecular weight of the PDMS matrix polymer on the HV outdoor insulation performance. Various RTV coatings with variable molecular weights of the units between crosslinks: 45,000- 28,000- 17,200- 9400 g/mol of PDMS were prepared using spraying on ceramic tiles. Coatings were characterized using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), Fourier transform infrared spectra (FTIR), Raman spectroscopy, surface wettability via contact angle measurements, and tensile strength was conducted to evaluate the physicochemical properties. Furthermore, inclined plane tracking (IPT) was performed to evaluate the erosion and tracking of the sprayed coatings. Results revealed that the highest molecular weight PDMS (45000 g/mol) showed four times longer IPT failure time with a lower erosion effect compared to PDMS coating of the lowest molecular weight (9400 g/mol). Moreover, coatings with the highest molecular weight depicted the highest contact angle, better mechanical properties, and enhanced thermal stability at high temperatures compared to their counterparts. Overall, our study showed that increasing the molecular weight between crosslinks results in better outdoor HV insulation performance. This fundamental study may open the avenue to develop a new generation of coatings with outstanding high voltage insulation upon coupling coatings of high molecular PDMS with different types of fillers.

EFFECT OF SUBSTITUTION OF PHOSPHONIC ACID BY CARBOXYLIC ACID IN POTENTIAL DRUG MOLECULES. A COMPUTATIONAL STUDY BENEFICIAL FOR PHARMACEUTICAL INDUSTRY

Syed Tahir Ali[1], Mansoor Kamal[1]

[1]*Department of Chemistry, Federal Urdu University of Arts, Science and Technology, Karachi, Pakistan*

Email: stahir.ali@fuuast.edu.pk

Many commercially important compounds are Phosphonic acid, Phosphonates, including Glycophosphate, the herbicide “Roundup”, and Ethephon, a widely used plant growth regulator. Bisphosphonates are popular drugs for treatment of osteoporosis. Carboxylic acids occur widely in nature and also present in the amino acids (which make up proteins) and acetic acid (which is part of vinegar and occurs in metabolism). Other than this, many medicines and pharmaceutical products contain carboxylic acid in their structure. Hence both Phosphonic and carboxylic acids have many applications in industry as well as in daily life.

The changes in physiological properties occur when a carboxyl group is substituted by a phosphonic group. Many experimental studies are present in literature which discuss these physiological changes [2-5]. In our present research work, we computed acid dissociation constant (pK_a) and partition coefficient (log P) values of different derivatives of Carboxylic acid Phosphonic acid to understand the behavior of both functional groups on physiological properties. This study is very helpful in finding the new potential molecules as drugs, because, pK_a and log P values are basic properties of a molecules to be used as drugs.

In this research work, a series of low molecular weight heterocyclic carboxylic and phosphonic acids are selected to compute pK_a and log P values. These values are compared to those of substituted benzene phosphonic acids, carboxylic acids, sulfonamides, and tetrazoles. This study has provide insight information of new potential drug molecules. The structures of some important compounds, which can serve as potential drugs are shown are in Figure 1 and 2. The computational results obtained through DFT method, B3LYP, are in reasonable agreement with the experimental once. This is concluded on the basis of correlation coefficient (R^2) and Mean Absolute Deviations (MAD) values.

EFFECTS OF A DUAL BIOPOLYMER SYSTEM ON THE OXIDATIVE STABILITY OF RED-PALM OLEIN-IN-WATER PICKERING EMULSION

See Kiat Wong,[1] Chien Lye Chew,[1,2] Tin Wui Wong,[3] Siah Ying Tang[1,4]

[1]Chemical Engineering Discipline, School of Engineering, Monash University Malaysia, Jalan Lagoon Selatan, 47500 Bandar Sunway, Selangor, Malaysia.
[2]Sime Darby Research, R&D Centre – Carey Island, Lot 2664, Jalan Pulau Carey, 42960 Carey Island, Selangor, Malaysia.
[3]Non-Destructive Biomedical and Pharmaceutical Research Centre, Smart Manufacturing Research Institute, Universiti Teknologi MARA, 42300 Puncak Alam, Selangor, Malaysia.
[4]Advanced Engineering Platform, School of Engineering, Monash University Malaysia, Jalan Lagoon Selatan, 47500 Bandar Sunway, Selangor, Malaysia.
E-mail: see.wong@monash.edu

Lipid oxidation remains an unresolved issue that decreases the nutritional value and quality of the food products, especially when the lipids are dispersed in aqueous phases, such as oil-in-water emulsions. It is well established that oxidation is initiated at the oil-water interphase where pro-oxidants come into contact with the lipids. Interest has recently been rising towards food compatible Pickering emulsions, a particle-stabilized emulsion system. Milk protein, sodium caseinate (SC), and cellulose nanocrystals (CNC) have proven to be strong candidates in forming a Pickering emulsion, and their physical stability has been reported. Yet, the combination of SC and CNC as Pickering stabilizers in lipid oxidation is mostly unexplored. Herein, we investigated the impact of different concentrations of CNC addition with 1% (w/v) SC and the control (without CNC) on the oxidation stability and physicochemical properties of an oil-in-water emulsion. During the accelerated stability test, the latter oxidized faster than emulsions stabilized by both SC and 1% (w/v) CNC, resulting in 26.7% and 19.5% higher amounts of primary and secondary lipid oxidation products, respectively. Moreover, the amount of free fatty acids was lowered by 28.9% with the addition of 1% (w/v) CNC. It was observed that the combination of polysaccharides with protein reduced lipid oxidation of emulsions, and the oxidative stability was found to be CNC concentration dependent. Furthermore, emulsion prepared at 1% (w/v) CNC showed the highest negative droplet surface charge (-53 ± 2.3 mV) as compared with the control (-35 ± 1.8 mV), resulting in stable emulsions with strong inter-droplet electrostatic repulsion. This study demonstrated that the addition of CNC to SC in forming emulsions effectively reduced lipid oxidation and improved the stability of the oil-in-water emulsion.

EFFECTS OF TRANSITION METAL DOPING ON THE EFFICIENCY OF ION-IMPRINTED MEMBRANES FOR LITHIUM RECOVERY

Najam us Sahar Riyaz,[1] Sifani Zavahir,[1] Leena Al-Sulaiti,[2] Dong Suk Han[1,3]

[1]*Center for Advanced Materials, Qatar University, P.O. Box 2713, Doha, Qatar*

[2]*Department of Math., Stat. and Physics, College of Arts and Sciences, Qatar University, Doha, Qatar*

[3]*Department of Chemical Engineering, College of Engineering, Qatar University, P.O. Box 2713, Doha, Qatar*

[1]*Email: ns.riaz15@gmail.com*

Lithium is the lowest density metal, very electrochemically active, and has the highest heat capacity out of all the metals. These distinct properties make lithium a precious commodity in the industry. With the growing popularity of electric vehicles and lithium-ion batteries, the demand for lithium in the industry has witnessed an exponential increase. However, the global industry is facing a lithium shortage as the increase in consumption of lithium (16%) has surpassed the increase of production (12%)[1], thus creating a supply vacuum in the market. In line with this trend, it is critical to focus on improving the processes of lithium production and refinement to avoid the impending lithium deficit. The cost inefficiency of the existing processes has left them out of the limelight, and several technologies are in dire need of improvement to ensure higher yields of lithium recovery[2].

The predominant categories of lithium recovery technologies include electrochemical methods and membrane-based technologies. However, both technologies have limited large-scale applicability due to high production costs and low stability. Considering this, ion-imprinted membranes (IIM) is an emerging research area for lithium recovery. Previous studies have shown that these IIM systems demonstrate almost twice the selectivity and greater than 90% efficiency levels in lithium recovery compared to electrochemical and other membrane-based methods. This study will explore the effects of different metal precursors as well as the effect of transition metal doping on lithium recovery efficiency using IIM.

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EFFICIENT DEGRADATION OF VARIOUS EMERGING POLLUTANTS BY RECOMBINANT FUNGAL DYP PEROXIDASES

Khawlah Athamneh[1], **Tuck Seng Wong**[2], **and Syed Salman Ashraf**[1]

[1]Department of Biology, College of Arts and Sciences, Khalifa University, Abu Dhabi, United Arab Emirates.
[2]Department of Chemical & Biological Engineering and Advanced Biomanufacturing Centre, University of Sheffield, Sir Robert Hadfield Building, Sheffield, United Kingdom.
Email: syed.ashraf@ku.ac.ae

The accumulation of emerging pollutants in the environment is a major concern as evidenced by an ever-increasing number of reports showing their adverse effects on environment and health. Hence, removal strategies of such pollutants remain an active area of investigation. A greener way by which these emerging pollutants can be eliminated from the environment is through enzyme-mediated bioremediation. Enzyme-based degradation can be further enhanced via advanced protein engineering strategies. Attempts to make efficiently express and purify recombinant plants peroxidases such as Soybean peroxidase and Horseradish peroxidase in *E. coli* have not been very successful. A better set of recombinant peroxidases to try instead could be fungal peroxidases. In the current study, we investigated the ability of four different recombinant fungal dye decolorizing peroxidases (DyPs) to degrade a panel of different emerging pollutants, using a previously developed sensitive and robust (LCMSMS)-based approach. Additionally, the role of a redox mediator was examined in these enzymatic degradation reactions. We showed that a subset of the tested emerging pollutants were efficiently degraded by these peroxidases, whereas others were recalcitrant. Addition of the redox mediator had a synergistic effect as it enabled complete degradation of additional emerging pollutants. Our results highlight the potential of fungal DyPs to be used for the bioremediation of different classes of emerging pollutants.

ELECTRICALLY SWITCHED ION EXCHANGE PROCESS BASED ON $LiAlO_2$ MATERIALS FOR HIGHLY EFFICIENT LITHIUM RECOVERY FROM SOLUTIONS

Sifani Zavahir,[1] Umme Hafsa,[1,2] Leena Al-Sulaiti,[3] Dong Suk Han[1,2]

[1]*Center for Advanced Materials, Qatar University, Doha, Qatar*
[2]*Department of Chemical Engineering, College of Engineering, Qatar University, Doha, Qatar*
[3]*Department of Math., Stat. and Physics, College of Arts and Sciences, Qatar University, Doha, Qatar*

E-mail: fathima.z@qu.edu.qa

The use of lithium (Li)-ion batteries in the fast-growing portable electronics and electric vehicle markets has created a huge demand for Li, and conventional solar drying is highly time-consuming, resulting in a vacuum in demand and supply. Electrically switched ion exchange (ESIX) technique has recently gained attention as an energy-efficient alternative that significantly reduces the Li ion concentration times from years to days or hours. In light of this, we report the successful synthesis of porous and scalable electroactive $LiAlO_2$ for the selective extraction of low concentrations of Li^+ ions. Li^+ ion adsorption capacity evaluation showed that more than 90% of the equilibrium adsorption capacity was achieved within 1 hour. Additionally, the system in operation confirmed the recovery of Li with 97% purity and specific energy consumption of 100Wh mol^{-1}. The $LiAlO_2$ electroactive film displayed evident selectivity for Li^+ ions at various Li^+/Na^+ and Li^+/Mg^{2+} ratios in simulated brine. $LiAlO_2$ also rendered superior electrochemical stability, and the normalized ion exchange capacity retention with only 5% loss of activity after 50 cycles of adoption-desorption operation. Due to the low ion transfer resistance and inherent ion pumping effect of ESIX, $LiAlO_2$ stands out as a promising and sustainable alternative to lithium manganese oxide (LMO) and $LiFePO_4$ for lithium recovery by ESIX technology.

ELECTROCATALYTIC OXIDATION OF METHANOL OVER SILVER BASED Ag-M/C (M=Cu, Zn, Fe, Cr, Mn) ELECTROCATALYSTS SYNTHESIZED BY SOLUTION COMBUSTION TECHNIQUE

Khulood Logade[#], **Sadiyah Shafath**[#], **Anand Kumar**[*], **Ibrahim Abu Reesh**[*]

Department of Chemical Engineering, College of Engineering, Qatar University, Doha, PO Box 2713, Qatar
 # Contributed equally

* *Corresponding author: akumar@qu.edu.qa; abureesh@qu.edu.qa; phone: (+974) 4403 4164*

Herein, we report the electrocatalytic properties of Ag-M/C (M=Cu, Zn, Fe, Cr, Mn) catalysts synthesized using solution combustion synthesis (SCS) method for methanol oxidation reaction (MOR). The morphological properties of the synthesized catalysts were studied using SEM, EDX, TEM, XRD and XPS techniques. The results indicated AgCu/C to be the most porous catalyst with small and well distributed nanoparticles making it a suitable choice for electrocatalytic applications. The XPS results showed a shift in peak in the AgCu/C sample due to the charge transfer between Ag and Cu indicating a strong interaction in the compound. The electrochemical measurements in 1M methanol with 1M KOH electrolyte by cyclic voltammetry (CV) and linear sweep voltammetry (LSV) revealed that AgCu/C shows greater electrocatalytic activity for MOR. Further studies on AgCu/C for methanol concentrations of 0.5 M, 1 M, 1.5 M, 2.5 M to evaluate the rate dependency of the catalyst indicated a power law dependency with an order 0.55 on methanol concentration. The catalyst also displayed long-term stability when chronoamperometry analysis was performed for 20 hours.

ENHANCED MEDICINAL PROPERTIES FROM THE SYNERGY BETWEEN TURMERIC AND BLACK PEPPER

Jian Hung Sam,[1] **Yen San Chan**[1]

[1]*Department of Chemical and Energy Engineering, Faculty of Engineering and Science, Curtin University Malaysia, 98000 Miri Sarawak*

Email: ivansjh@postgrad.curtin.edu.my, chanyensan@curtin.edu.my

Turmeric and black pepper are excellent food choices that are usually used together in many cooking recipes. Research has shown that the combination of these two spices produces synergy and grants enhanced properties when it comes to human health and nutrition. Special synergical effects, such as improved antioxidant, anti-inflammatory, bioabsorption, bioavailability and so on, can be produced when the cumulative bioactive constituents of two natural plant extracts come together, introducing more diverse constituents which contributes to higher potential of enhanced properties. The purpose of this study was to evaluate the antioxidant activities of turmeric, black pepper and its combination using 1,1,-Diphenyl-2-picrylhydrazyl (DPPH) assay. Turmeric and black pepper extract showed antioxidant activity of 10.80% and 2.03% respectively, while in combination the two extracts exhibited 6.63% which is higher than the expected result of 6.42%. The results obtained are in line with various research and contributes to one of the many synergistic effects between black pepper and turmeric. Other than the enhancement of antioxidant activity, the two spices are used concurrently mainly for their pharmacological synergy in specific medicinal treatments and as a nutraceutical which stem from the mechanisms from the mixture of bioactive constituents in both the spices. This presentation explores the scientific evidence behind the interaction of turmeric and black pepper and it's improved properties exhibited *in vitro* and *in vivo*. The in-depth bioactive constituents responsible for synergism between the two extracts will also be reviewed. Turmeric and black pepper are only one pair of natural plants that exhibit synergism, with nature granting us a library of natural products, this prompts more research into discovering and understanding the potential combinations between natural products, looking for potential synergy.

Keywords: Turmeric, Black Pepper, Synergy, Plant, Food

ENHANCED STABILITY AND PHOTOLUMINESCENCE QUANTUM YIELD OF CESIUM LEAD BROMIDE PEROVSKITES BY HEXADECYLTRIMETHYLAMMONIUM BROMIDE DOPING

Christina Al-Tawil[1], Riham El Kurdi[1], Digambara Patra[1]

[1]*Department of Chemistry, American University of Beirut, Beirut, Lebanon*
Email: cea22@mail.aub.edu

Perovskites nanoparticles having a crystalline structure have attracted scientists' attention due to their great potential in solar cell applications and various other fields ranging from chemical and industrial to biomedical used. Unfortunately, cesium lead halide perovskites suffer from their high instability, where they undergo a rapid chemical decomposition within time. For this purpose, here three different reaction parameters have been varied starting from the time of the reaction, concentration of lead bromide, and concentration of cesium oleate during preparation of $CsPbBr_3$ pervoskite nanoparticles. Furthermore, the prepared perovskites have been characterized using UV-Visible absorption spectroscopy, fluorescence spectroscopy, scanning electron microscopy, thermogravimetric analysis and X-Ray diffraction technique. It is found that the most stable $CsPbBr_3$ were formed when mixing 0.15 g (C= 0.06812 M) of lead bromide heated for 40 minutes, with a volume of 1.2 mL of cesium oleate. Subsequently, after the successful preparation of $CsPbBr_{3,}$ hexadecyltrimethylammonium bromide (CTAB) is used as an ecofriendly surfactant dopant in order to test in the first place; the stability of the formed perovskites, and later on to boost their photoluminescence quantum yield (PLQY), which have not been explored in literature. Results show CTAB as dopant enhances efficiency of the formed $CsPbBr_3$ nanoparticles by increasing their stability remarkably and enhancing PLQY up to 75%.

ENHANCING THE PERFORMANCE OF PHOTOVOLTAIC (PV) PANELS USING ANTI-SOILING COATINGS TECHNIQUES

Enas Fares,[1] Rima Isaifan,[1]

[1] Division of Sustainable Development, College of Science and Engineering, Hamad Bin Khalifa University, Qatar Foundation, P.O. Box 5825, Doha, Qatar
E-mail: efares@hbku.edu.qa

Global interests are shifted from conventional energy sources towards renewable ones. Extensive research is implemented under Photovoltaic (PV) solar energy, especially in the Gulf region due to the high solar irradiance. However, one of the main drawbacks in the region is the accumulation of dust on the PV panels, which degrade the power output of the PV modules radically (e.g., a daily average of -0.41 % of energy yield at the Solar Test field facility of QEERI). This study aims to understand the soiling mechanisms and develop an anti-soiling coating effective against dust accumulation and can maintain the PV module's efficiency. Many studies tackled such a problem focusing on polymers, SiO_2, and TiO_2 materials using mainly two deposition techniques: dip and spin coating.

Consequently, this study will contribute to the knowledge by using one of the contemporary deposition techniques: inkjet printing, to deposit metal oxide inks to form a textured anti-soiling thin film over the glass substrate to help, if not eliminate, the dust accumulation. Furthermore, the novelty is not only on using inkjet printing but also on combining and comparing different textures and different metal oxides such as TiO_2, Al_2O_3, SnO_2, and ZnO for the purpose of PV anti-soiling application. The reason for selecting metal oxide materials is their mechanical and chemical stability and reliability. Moreover, the inkjet printing technique is easy to scale up and (provides a high control on the formed pattern, which allows the researcher to test different texturing of the deposited thin films and their relation in enhancing the anti-soiling properties. The experimental part of this thesis has utilized two types of inks; (1) the mixed metal salts with metal oxide nanoparticles and (2) the pure metal oxide nanoparticles. This work also reports on the optical and morphological properties of various inorganic metal oxide compounds deposited by the newly developed inkjet printing processes for their field assessment for anti-soiling applications over solar panels. Four inorganic metal oxides were selected for this study, namely TiO_2, Al_2O_3, ZnO, and SnO_2, due to their proven physico-chemical properties such as the wide bandgap, self-cleaning ability, mechanical stability, and anti-reflectivity, which are all needed for anti-dust applications.

UV-Vis spectroscopy, total transmittance (TT), and total reflectance (TR) were systematically investigated. Field emission scanning electron microscope, X-ray diffraction, and X-ray photoelectron spectroscopy measurements were carried out to probe these thin films' structural, morphological, and chemical properties. Contact angle measurements were then obtained to assess the hydrophobicity of the coatings. Finally, our developed methods based on nanoparticles-ink and mixed-based-ink will be tested outdoor to assess the anti-soiling properties. Our results showed that the substrate's transmittance using nanoparticles (NP)-ink revealed better optical properties than the mixed-based-ink. This optical enhancement might be due to NP's voids, which reduce the spectra scattering and deterioration and, thus, have better optical properties. A homogeneous layer is observed in all samples with dense NP in ZnO, TiO_2, and SnO_2 NP and mixed inks. The contact angles were found to be ranging between 8.5^o to 47.8^o, thus indicating that the synthesized films are hydrophilic/super-hydrophilic coatings. The samples were tested for soiling outdoor for 22 days to assess their anti-soiling properties under real conditions. The outdoor test revealed that Al_2O_3, ZnO, and TiO_2 are promising materials for anti-soiling coating applications for both ink types.

EVALUATION OF NUTRITIONAL CONSTITUENTS OF MONKEY KOLA *Cola millenii* SEED AND PULP.

Ayowumi Modupe APOESO, Muibat Olabisi BELLO, Tolulope Ademuyiwa BABALOLA

Department of Pure and Applied Chemistry,

Ladoke Akintola University of Technology, Ogbomoso, Nigeria.

E-mail of corresponding author: apoesoayowumi@gmail.com

There is an increasing demand and focus on plants food as major component of human diets and this can be attributed to the several health benefits that is attached to the consumption of plants food. Due to the increasing demand on valuable foods with essential nutrients, need for higher agricultural production and research into full potential of several species of local agricultural crops that abound in developing countries but are underutilized are required. One of this less familiar plant of the wild is *Cola millenii* k. schum, which is commonly known as monkey kola in English, atewo edun or obi edun by Yoruba speaking people, achiokokoro by Igbo speaking people.

Cola millenii is a tree with an average height of 12metres or sometimes more and the name monkey kola is gotten from its relish by primate animals. It belongs to the Steruliaceae family and it is commonly found in the deciduous, closed and transition forest of Southern Nigeria. The seed and pulp of *Cola millenii* was analyzed to establish its nutrient constituents in order to investigate the possibility of using them for human and animal consumption.

The proximate analysis was done using Association of Analytical Chemists, AOAC method, minerals quantification using Atomic Absorption Spectrophotometer, amino acids using high performance liquid chromatography, viscosity using automated brookfield viscometer model LV. Proximate constituents of *Cola milleni* seed and pulp were: 14.88 and 6.56% crude protein, 4.02 and 10.53% crude fibre, 0.01 and 4.01% ash, 4.01 and 2.03% lipid, 8.02 and 14.01% moisture and 69.06 and 62.86% carbohydrate. Viscosity increases with increase in temperature for pulp, seed and seed cake. The amino acid profile reveals the presence of 8 essential amino acids and 9 non-essential amino acid. Glutamic acid was the highest while cysteine was the lowest amino acid present in the seed sample. Mineral composition showed sodium to be the most abundant in both the seed and seed cake (1.56 ± 0.02mg/kg and 1.35 ±0.02mg/kg) while cadmium was the least abundant in the seed and seed cake (0.01 ± 0.00mg/kg).

The seed and pulp of *Cola millenii* contain appreciable amount of nutrients and minerals, which are nutritional requirements of both humans and livestock. This suggest that the seed and pulp could be useful as feed supplement to improve health and growth performance.

Evaluation of the Influence of the Eggshell Content on the In-vitro Biodegradation Behavior of Mg-2.5 Zn/Eggshell Composite Materials in Simulated Body Fluid

Bahgat Radwan[a], Paul C. Okonkwob[b], Srinivasan Muruganb[b], Maryna Tarybac[c], M. Fatima Montemorc[c], Layla Al-Mansoorid[d], Mohamed A. Elrayess[d], Noora Al-Qahtania[a], Gururaj Parandee[e], Manoj Gupta[e], Khaled M. Youssef[f], Raymundo Case[g], R.A. Shakoor[a], and Aboubakr M. Abdullah[a,*]

[a] Center for Advanced Materials, Qatar University, P.O. Box 2713, Doha, Qatar
[b] Department of Mechanical and Mechatronics Engineering Dhofar University Salalah Oman
[c]Centro de Quimica Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
[d] Biomedical Research Center (BRC), Qatar University, Doha, Qatar
[e] Department of Mechanical Engineering, National University of Singapore, 9 Engineering Drive 1, Singapore 117576, Singapore
[f] Department of Materials Science and Technology, Qatar University, Doha, 2713, Qatar
[g] Department of Materials Science and Engineering, Texas A&M University, College Station, TX, 77843, USA

Biodegradable magnesium alloys have been considered a promising alternative solution for non-permanent implants, such as cardiovascular-related applications, and the construction of orthopedics devices. In this work, zinc (Zn) and eggshell (ES) reinforced biodegradable magnesium alloy (Mg–2.5Zn) were used as environment conscious (eco) composite (Mg–2.5Zn–xES). The composite was obtained employing the disintegrated melt deposition (DMD) technique. In vitro tests were conducted to explore the effect of the concentration of ES (3 and 7 wt.%) on the biodegradation behavior of the Mg–Zn alloys in simulated body fluid (SBF) at 37 °C. The corrosion behavior of the Mg–2.5Zn–xES composites was studied using different techniques such as weight loss measurement, hydrogen evolution, potentiodynamic polarization, electrochemical impedance spectroscopy (EIS), and Scanning Vibrating Electrode Technique (SVET). The outcomes indicated that Mg–2.5Zn–3ES possesses the lowest degradation activity. The surface morphology and the composition of the degraded surfaces were explored by X-ray diffraction (XRD), scanning electron microscopy (SEM) coupled to energy-dispersive X-ray spectroscopy (EDS), and X-ray photoelectron spectroscopy (XPS).

Keywords: Magnesium alloy; Metal Matrix Composite; Biodegradable; SBF; cytotoxicity, localized corrosion; SVET.

FATTY ACIDS IN THERMOPHILIC CYANOBACTERIA

Fong Li Yee[1], Nur Izzati Mohd Noh[2], Anthony Nyangson Steven[1]

[1]Department of Chemistry, Faculty of Science, University Teknologi Malaysia, 81310 Johor Bahru, Malaysia
[2]Department of Biosciences, Faculty of Science, University Teknologi Malaysia, 81310 Johor Bahru, Malaysia
Email: anthony@utm.my

Thermophilic cyanobacteria, as photoautotrophic organisms, possess the metabolism to transform climate-damaging carbon dioxide (CO_2) to biomass with light as energy source and they are growing optimally in extreme environment [1]. This ability makes them to promising green cell factories for a more sustainable production of useful molecules [2]. Strains of thermophilic cyanobacteria were cultivated, the product produced were harvested and extracted. The determination of fatty acids and polyhydroxyalkanoates (PHA) composition were performed using gas chromatography mass spectrometer (GC-MS). Both fatty acids and PHA produced were found to be dependent on the nitrogen concentration.

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FAUX-DATA INJECTION OPTIMIZATION APPROACH FOR EXPEDITING MATERIALS DISCOVERY

Abdul Wahab Ziaullah[1], Sanjay Chawla[2], and Fedwa El-Mellouhi[1]

[1] Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. BOX 34110,Doha,Qatar
[2] Qatar Computing Research Institute, Hamad Bin Khalifa University, Doha P.O. Box 34110

E-mail: {awahab,felmellouhi,schawla}@hbku.edu.qa

Machine learning (ML) methods are now extensively being used to optimize and discover new materials by enabling us to predict newer molecular substitutes and optimal compositions of materials with desirable properties. Most ML models rely on datasets of various classes of materials to yield predictions on either the same (interpolation) or different (extrapolation) classes of materials. Robust models to automatically extract discriminatory features is the essential requirement for such ML models. It is well known that there are gaps in the data repositories pertaining to materials science, such that even state-of-the-art ML models trained on these data sets results in extrapolation errors that are outside acceptable error bounds for material selection. Moreover, refining the ML models by obtaining new data via physical experiments or Density Functional Theory (DFT) calculations can be time-consuming with traditional sequential optimization techniques. Assuming availability of multiple computational resources, traditional techniques might not be able to fully leverage them due to sequential execution bottleneck of typical data acquisition optimization methods such as Bayesian optimization (BO). Here, we tackle such bottleneck of BO and maximize the usage of available computational resources through a batch optimization technique based on faux-data injection in BO loop and determine k-candidates to run k-DFT computations on k-compute nodes, thereby expediting the discovery of materials. We utilize Organic-Inorganic Halide Perovskites for case study as the optimality of the results can be easily verified from the results of our previous works [1,2] and additionally, we compare our batch optimization strategy against baseline monte-carlo methods such as multiple random sampling and Particle Swarm Optimization.

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First-Principles Characterization and Experimental Validation of the Solid−Solid Interface in a Novel Organosulfur Cathode for the Li−S Battery

Satyanarayana Bonakala [1], Amar Deep Pathak [2], Alexey Deyko [3], Christina Christova [3], Indranil Rudra [2], Guy Verbist [4]

[1]*Qatar Environment and Energy Research Institute, Hamid Bin Khalifa University;* [2] Shell India Markets Pvt. Ltd, Bangalore 562 149, India. [3]PTG Eindhoven BV, 5612 AR Eindhoven, Netherlands.; [4]Shell Global Solutions International B.V., The Hague 2596 HR, Netherlands.

Email: Indranil.Rudra@shell.com

ABSTRACT[1]

Lithium-sulfur (Li−S) batteries store nearly twice as much energy per kilogram as the Li ion that shed light on commercial usage of batteries in heavy vehicles. Organosulfur silanes grafted on an aluminum current collector have been proposed and demonstrated to function as a sulfur source in the cathode for a lithium-sulfur (Li-S) battery. Bis[3-(triethoxysilyl)propyl]disulfide silane (TESPD) and bis[3-(triethoxysilyl)propyl]tetrasulfide silane (TESPT) are typical examples of organosulfur complexes used for the study. These organosulfur silanes act as an insulator. Formation of polysulfides (Li_2S_x), which is a major bottleneck in the case of elemental sulfur, can be eliminated using this novel cathode. In the absence of charge-carrying polysulfide species, the role of insulating TESPD/TESPT in the charge conduction pathway is an open question. Insight into the interface between the Al current collector and grafted TESPD/TESPT at an atomic level is a prerequisite for addressing the charge conduction pathway. The systematic theoretical methodology is developed based on electronic structure calculations and ab initio molecular dynamics simulations to propose the realistic cathode model (hydration environment) for the Li-S battery. A cluster model is developed to predict the reduction potentials of TESPD/TESPT disclosing the reduction reaction with Li, resulting in the intramolecular S-S bond breaking which is validated by experimental cyclic voltammetry measurements. A realistic cathode model between the aluminum current collector and TESPD/TESPT is also proposed to mimic the experimental conditions where the Al surface was exposed to O_2 and H_2O. The top few layers of Al are transformed into α-Al_2O_3 and covered with H_2O molecules in the vicinity of grafted TESPD/TESPT. The structural models are further validated by comparing simulated S 2p binding energies with experimental X-ray photoelectron spectroscopy studies.

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Functionalized Porous Metal-Organic Frameworks (Porous-MOFs) for Carbon Dioxide Capture

Palani Elumalai[a], Stefano Sanvito[b], Wolfgang Schmitt[c] and Fedwa El Mellouhi[a]

[a]Qatar Environment and Energy Research Institute (QEERI), Hamad Bin Khalifa University (HBKU), Doha, Qatar.

[b]School of Physics, Advanced Materials and Bioengineering Research Centre (AMBER) and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN) Institute, Trinity College, Dublin 2, Ireland

[c]School of Chemistry and SFI AMBER & SSPC Research Centres, University of Dublin, Trinity College, Dublin 2, Ireland

Email: epalani@hbku.edu.qa (P.E.) and felmellouhi@hbku.edu.qa (F.E.)

The class of porous materials like Metal-Organic Frameworks (MOFs) or mixed matrix materials (MMMs) are defined by supramolecular self-assembly of metal-core and organic spacers coordination networks has several advantages such as high surface area, and larger-pore.[1] The functionalized porous metal-organic frameworks (Parous-MOFs) have shown promising application in the capture of CO_2 from industrial tail gas and in low concentrated atmospheric condition.[2] In this work, we propose to use functionalized MOFs supported porous solids for the selective CO_2 capture from air, its storage and regeneration. The core-MOFs are synthesized from cheap reactants and functionalized to obtain the large surface area and pore-volumes owing to the presence of abundant flexible nanopores. A series of functionalized MOFs porous materials were thus prepared by post functionalization then characterized. We will discuss the research outcome of materials stability in different environments conditions such as in different time duration, temperature, moisture, acetic and base conditions. Preliminary results of CO_2 capture, regeneration and selectivity will be highlighted.

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GREEN SYNTHESIS AND CHARACTERIZATION OF CELLULOSE ACETATE FROM MAIZE HUSK

Eunice E. Okon[1], Nsinem E. Efiong[1]

[1]Dept. of Chemistry, Faculty of Science, University of Uyo, Uyo, Nigeria

unice.edet@gmail.com

Maize husk was used as raw material for synthesis of cellulose acetate by using a simple and efficient method. Cellulose was isolated from maize husk using standard pretreatment method with dilute alkaline and acid solutions and bleaching with 3% hydrogen peroxide. Cellulose acetate was synthesized successfully with the yield of 69% in presence of acetic anhydride and iodine as a catalyst. The extent of acetylation was evaluated from percentage yield and the degree of substitution (DS), which was determined by 1H NMR and titrimetrically. The synthesized products were characterized using FT-IR, 1H NMR and XRD.

GREEN SYNTHESIS OF ISATIN KETAZINES DERIVATIVES BY MONTMORILLONITE-H$^+$ AS ACID ECO-FRIENDLY HETEROGENEOUS CATALYST

Boumadiene Benlahreche[1] , Assya Taleb[1] , Mokhtar B. Lahrech[2] and Salih Hacini[1]

[1] Laboratoire de Chimie Fine (L.C.F), University Oran1, BP-1524-Menouar,31000- Oran, Algeria
[2] Laboratoire de Chimie Organique et Subst.Nat (LCOSNa), University of Djelfa, Algeria
E-mail: assyatab@yahoo.com, s_hacini@hotmail.com

In recent years, clay minerals have become a topic of discussion in many publications. In order to design clean or "green" chemical transformations, they can catalyze a variety of organic reactions occurring on their surface and interstitial space. In our study we were interested in the application of Algerian montmorillonite clay (MMT-H +) as green catalyst in synthesis of isatin ketazines derivatives. These structures possess a broad variety of biological and pharmacological properties. They also widely used as starting materials for the synthesis of a broad range of various heterocyclic compounds. [1]

The products were obtained in two catalyzed steps under conventional heating in ethanol. Treatment of isatin derivatives with hydrazine monohydrate gave isatin-hydrazone derivatives which were reacted with the appropriate aromatic ketones to obtain the desired compounds in good yields.

The montmorillonite-H$^+$ (MMT-H$^+$) was found to be an efficient green heterogeneous acidic catalyst for the synthesis of isatin ketazines derivatives. This catalyst was easy to prepare, environmentally friendly, highly stable and can be recycled without significant loss of activity. The distinguished advantageous of present synthetic method are use of inexpensive catalyst, simple reaction workup, good yields and reusability of catalyst. Other applications of this catalyst in synthetic processes are under study. [2]

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GREEN SYNTHESIS OF SILVER NANOPARTICLES USING *PSEUDOCALYMMA ELEGANS* LEAF EXTRACT (PE-AgNPs): A NEW HIGHLY SELECTIVE METHOD FOR COLORIMETRIC DETECTION OF LEVOFLOXACIN IN TAP WATER AND HUMAN PLASMA

Faiqa Ahsan[a], Tasneem Zehra[a,b], Muhammad Ali Versiani[a*],Sana Wahid[a], Syed Waseem Ahmed[a], Qandeel Laraib[c], Maryam Shafique[d], Sehar Afshan Naz[d], Sajid Jahangir[a], Muhammad Raza Shah[e], Shaheen Faizi[e]

[a]*Department of Chemistry, Federal Urdu University of Arts, Science & Technology, Karachi, Pakistan*

[b]*Department of Basic Science & Humanities, Dawood University of Engineering & Technology, Karachi, Pakistan*

[c]*Department of Biosciences, Mohammad Ali Jinnah University Karachi, Pakistan*

[d] *Department of Microbiology, Federal Urdu University of Arts, Science & Technology, Karachi, Pakistan*

[e]*H.E.J. Research Institute of Chemistry, International Center of Chemical and Biological Sciences, University of Karachi, Karachi, Pakistan*

Email: faiqa.qureshi628@gmail.com

mail.versiani@fuuast.edu.pk

Abstract

This study focuses on the rapid and feasible formation of silver nanoparticles (AgNPs) by a new source *Pseudocalymma elegans* (PE) leave extract. The characterization of PE-AgNPs was done by AFM, DLS, EDX, FTIR, SEM, and UV-Vis techniques. The appearance of yellow color indicated the formation of AgNPs and further confirmed by surface plasmon resonance (SPR) peak at ~ 412 nm. The average size of synthesized AgNPs were approximately 22-55 nm with spherical in shape. FTIR spectrum revealed the functional groups which were present in PE leave extract, and responsible for the reduction, capping, and synthesis of PE-AgNPs including alcohols, carbonyl, and phenol. PE-AgNPs were able to recognize levofloxacin (LV) selectively with consequential increase in the absorbance at 412 nm. The analytical properties of PE-AgNPs were observed via changing the concentrations of LV that obeyed Beer's law within the range of 01 to 1000 μM ($R^2 = 0.972$). The limit of detection (LOD) was equal to 108 μM. Moreover, Antibacterial potential of synthesized PE-AgNPs was also determined and good inhibitory activities were observed towards Gram-negative bacteria specifically *Pseudomonas aeruginosa* (ZI = 16.3 ± 0.9 mm, MIC = 0.175 mg/mL) as compared to standard drugchloramphenicol (ZI = l9.0 ± 0.8 mm). These AgNPs could provide novel economical biosensors to detect the pharmaceutical drug (levofloxacin) in various samples and may also play a significant role in the fabrication of nano-based antibacterial drugs in near future.

Keywords

Silver nanoparticles; *Pseudocalymma elegans*; Levofloxacin; Colorimetric detection; Antibacterial activity; economical biosensors.

HIGHLY ACTIVE MULTIFUNCTIONAL LANTHANUM PEROVSKITE ELECTROCATALYSTS ($LaMn_xCo_{1-x}O_3$ ($0 \le x \le 1$)) BY TUNING THE Mn TO Co RATIO IN ALKALINE MEDIUM

Sadiyah Shafath[#], **Khulood Logade**[#], **Anchu Ashok, Anand Kumar**[*], **Ibrahim Abu Reesh**[*]

Department of Chemical Engineering, College of Engineering, Qatar University, Doha, PO Box 2713, Qatar
 # Contributed equally

** Corresponding author: akumar@qu.edu.qa; abureesh@qu.edu.qa; phone: (+974) 4403 4164*

Lanthanum-based perovskites ($LaMn_xCo_{1-x}O_3$ ($0 \le x \le 1$)) were synthesized using a solution combustion synthesis technique with variable ratios of Co and Mn to investigates the surface property and electrocatalytic characteristics (stability and activity of catalyst) for methanol oxidation reaction (MOR), oxygen reduction reaction (ORR), and oxygen evolution reaction (OER) under alkaline medium (KOH). The structural, chemical and morphological characterizations of the synthesized catalyst were performed by XRD, FTIR, SEM, TEM and XPS techniques as a function of Mn:Co elemental ratio. The time temperature profile during combustion process was also monitored to study the completion of combustion reaction and to understand its impact on the structure of the perovskites. SEM/EDX and XPS analysis confirmed the formation of targeted ratio of Mn and Co on the catalyst. Cyclic voltammetry (CV) and linear sweep voltammetry (LSV) results revealed that all perovskite samples with different Mn:Co ratios were active for ORR, OER and MOR. The $LaMn_xCo_{1-x}O_3$ perovskite with $x=0.4$ showed the highest current density compared to the other samples towards all the electrocatalytic reactions under alkaline reaction conditions.

HOW DOES CHANGE IN TYPE OF ABSORPTION MEDIUM (BARIUM HYDROXIDE OR CALCIUM HYDROXIDE) AFFECT THE ABSORPTION RATE OF CARBON DIOXIDE

Ibrahim Abdulrahman Al Hoori, Sunny Joseph

Qatar Leadership Academy, Qatar

sjoseph@qf.org.qa

Recurrence of ice age and climate change have been happening many times in our planet's history. Significant and widespread impacts are visible on Earth's atmosphere due to climate change on a global scale. In the previous centuries, human impact to this change was minimal. However, in the recent times, it has been increasing many folds. Climate change is the change in climatic patterns in different areas around the world. Methane, nitrous oxide, fluorinated gas etc. causes global warming. However, carbon dioxide is the main culprit here. It is produced primarily by the burning of fossil fuels and wild fires. Deforestation adds carbon dioxide to the atmosphere, while forest reforestation removes it.

According to Hannah Ritchie, head of Research at Our World in Data.org, In Qatar's CO2 emissions in 2017 were 49.7 tons per person. In Chad, only 0.04. (1 person of Qatar= 1243 people of Chad). As per her research, strong reliance on fossil fuels. Resource-intensive lifestyles, water desalination, high air conditioning consumption etc. are the cause of this emission. The average temperature in Qatar has gone by two degrees. It is imperative that we need to tackle this formidable problem so that we can reduce our impact on climate change. The research question is "How does change in type of absorption medium (Barium hydroxide or calcium hydroxide) affect the absorption rate of carbon dioxide?".

The method involves modeling an experiment in the lab that could be conducted outside. A stream of carbon dioxide is prepared in the lab by reacting NAHCO3 with Acetic acid. $Ba(OH)_2$ and $Ca(OH)_2$ filters ware prepared and are exposed to carbon dioxide gas in the lab. Then the amount of CO2 felted through the filter are measured using a Vernier CO2 sensor. The values are compared with a control (filter with no chemicals). The results are analyzed to check the efficacy of the filters. The results are further confirmed by weighing the CaCO3 produced on filter papers before and after reaction.) It is seen that both filters are able to absorb CO_2 and take it away from the air. However, $Ba(OH)_2$ demonstrates a superior ability to absorb CO_2.

It is suggested that these materials can be used to be pasted on appropriate filters and mounted along the Al Shamal road or other highways so that the exhaust from the vehicles can be captured. The produced carbonate (a solid) can be scraped off and be converted to other useful products. The method can be used near oil refineries or other busy places like football stadiums. By incorporating this method with other carbon foot print reducing techniques, we may be able to reduce the "Average - Doha temperature" by at least 10c by the end of 2025. In long run, further reduction in temperature is possible. Hopefully by educating the public about global warming and its effect on Doha, we may be able to energize the public to take part in the reversal of this trend.

IMPROVING THE MECHANICAL PROPERTIES OF SOLUTION BLOWN SPUN NANOFIBER MEMBANRS BY HEAT-PRESS POST-TREATMENT

Arqam Azad Shahab, Hammadur Rahman Siddiqui, Haleema Saleem, Syed Javaid Zaidi*

UNESCO Chair for Desalination and Water Treatment,
Center for Advanced Materials (CAM), Qatar University, Qatar
**E-mail address: szaidi@qu.edu.qa*

Nanofibers are complicated fiber networks with a nanoscale diameter, with high porosities and well-connected pore frameworks. Out of the different nanofiber fabrication techniques, the solution blow spinning (SBS) method has received more research interest, relative to standard electrospinning technique due to its easy operation, higher production rate of nanofibers, and non-requirement of high-voltage electrostatic field support such that the process safety is comparatively more [1]. Despite the numerous benefits of SBS technique, it has certain disadvantages like poor mechanical properties, poor fiber morphology, and larger pore sizes, limiting the application of SBS nanofiber membranes for various applications such as membrane-based water treatment. Considering this, in the present study, we establish a method of fabricating morphologically improved and strong polymer-based nanofiber membranes (NFMs) using the advancing SBS technique and a subsequent heat press post-treatment.

In this study, polyether sulfone (PES) solutions with two distinct concentrations (25 and 20 wt.%) in N-methyl-2-pyrrolidone (NMP)/toluene solvent mixture (2:1 wt.) were solution blown spun at 5.0 ml/h feed rate, 2.0 bar air pressure, deposition time 10 min, and a varying voltage. The membranes prepared were hot-press treated at varying temperatures, different pressing times, and under varying load, and a great improvement in morphology and mechanical properties were noted. The data and results consistently showed a significant increase in overall mechanical properties of the nanofiber mats. Additionally, the DMA results of the modified membranes demonstrated good thermal stability. The NFMs of the current invention demonstrated smoother surface following the heat-press post treatment, relative to the base samples Moreover, the fiber mats can be optimized in terms of pore diameter and material used, as well as the type of post processing used, depending on the application. Additionally, the NFMs of the current invention demonstrated smoother surface following the heat-press post treatment, relative to the base samples. Furthermore, the heat-press post treatment can result in a decreased pore size, which would be advantageous for different NFM applications like water treatment filters, aerosol filtration, battery separators, textile membranes, protective clothing, and protective masks.

Acknowledgements

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IMPROVING THE THERMAL CONDUCTIVITY AND PHOTOTHERMAL CONVERSION PERFORMANCE OF PARAFFINS/POLYETHYLENE PHASE CHANGE COMPOSITE USING EXPANDED GRAPHITE

Safna Nishad*, Patrik Sobolciak and Igor Krupa*,

Center for Advanced Materials, Qatar University, P.O. Box 2713, Doha, Qatar
E-mail: sn1518223@qu.edu.qa (S. Nishad); igor.krupa@qu.edu.qa (I. Krupa)

Abstract

Solar energy harvesting has gained much attention by researchers to switch towards a renewable energy source considering its vast and abundant availability. The solar thermal collectors harvest direct heat or photothermal energy to use for space and water heating. However, its intermittent availability necessitates an associated thermal energy storage system to provide a continuous energy supply. Therefore, recent studies focus on latent heat storage systems using phase change materials (PCMs) for thermal energy harvesting and storage. PCMs store the excess thermal energy during the off-peak load period and recover it when the supply is limited. Among various PCMs, paraffins are widely studied due to their large latent heat, non-corrosiveness, good thermal and chemical stability. Shape instability during phase change, low thermal conductivity, and lack of photoabsorbance are the major drawbacks of paraffins. Therefore, shape-stabilized phase change composites (SSPCC) were fabricated in this study by hot pressing the mixture of paraffin, polyethylene, and expanded graphite (EG) to overcome the above limitations. The addition of polyethylene provided shape stability and increased the thermal conductivity of paraffins by 90%. Further addition of EG enhanced the thermal conductivity of the composite by 300% with 10% (by weight) of EG in the composite. Moreover, the excellent photoabsorption of EG effectively converted the photo energy to thermal energy and stored it as latent heat by paraffins in the composite. The fabricated SSPCMs with 10% of EG exhibited 61% of photothermal conversion and storage efficiency and which is promising for solar thermal conversion and storage applications.

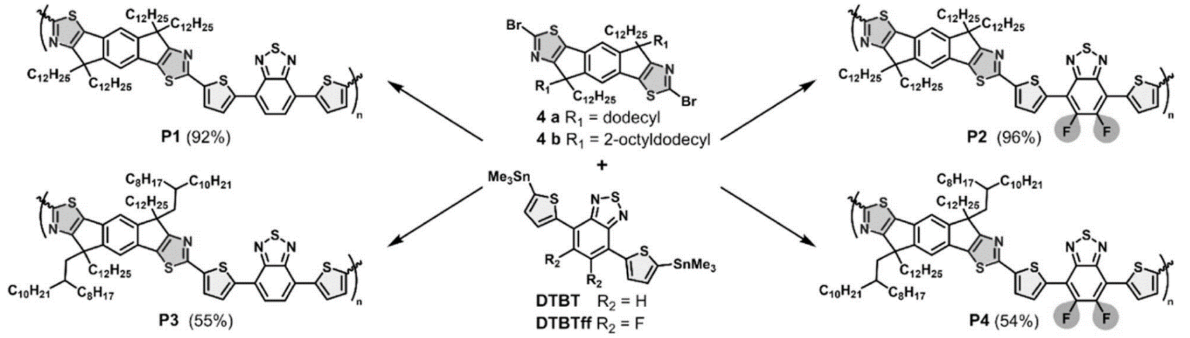
Acknowledgment: This work was supported by the Qatar National Research Fund through the award NPRP13S-0127-200177.

INDACENODITHIAZOLE LADDER BASED CONJUGATED COPOLYMERS FOR AMBIPOLAR OFET APPLICATIONS.

M. Barłóg,[1] **X. Zhang,**[2] **I. Kulai,**[1] **D. Sredojevic,**[1] **A. Sil,**[3] **X. Ji,**[4] **K. S. M. Salih,**[5] **H. S. Bazzi,**[1] **H. Bronstein,**[6] **L. Fang,**[4] **T. J. Marks,**[3] **X. Guo** [2] **and M. Al-Hashimi***[1]

[1] *Department of Chemistry, Texas A&M University at Qatar P.O. Box 23874, Doha, Qatar*
[2] *Department of Materials Science and Engineering, Southern University of Science and Technology, Shenzhen, China*
[3] *Department of Chemistry and the Materials Research Center, Northwestern University, Evanston, IL 60208-3113, USA*
[4] *Department of Chemistry, Texas A&M University, College Station, TX 77845, USA*
[5] *Department of Chemistry and Earth Sciences, Qatar University, P.O. Box 2713, Doha, Qatar*
[6] *Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, United Kingdom.*
Maciej.barlog@qatar.tamu.edu

Several conjugated copolymers based on the electron-rich indacenodithiophene (IDT) and its analogues donor units have afforded impressive high mobilities due to the enhanced inter-chain interactions facilitating the coplanarity of the polymer backbone. We demonstrated that replacing the flanking thiophene units with electron-deficient thiazole cores increases the electron affinity, stabilizing energy level with enhanced both inter-chain π−π interactions and intra-chain π-conjugation. This structural adjustment allowed convenient shifting from the p-type charge transfer typical for IDT into ambipolar characteristics for IDTz based polymers.



INFLUENCE OF SYNTHESIS PROCEDURE ON THE CATALYTIC PERFORMANCE OF COPPER NANOPARTICLES-SUPPORTED CERIA TOWARDS CATALYTIC OXIDATION OF CARBON MONOXIDE

Alaa Elsafi,[1] Muna Ibrahim,[1] Yahia H. Ahmad,[1] Assem T. Mohamed,[1] Aymen Abu Hatab,[1] Siham Alqaradawi[1]

Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University, Doha 2713, Qatar
E-mail: aa1702336@qu.edu.qa (A.E.); mi1701758@qu.edu.qa (M.I.); yahiashoeb@qu.edu.qa (Y.A); assem.m@qu.edu.qa (A.M); aymenabuhatab@hotmail.com (A.A); Siham@qu.edu.qa (S.A)

It is evident that the synthesis approach has a remarkable effect on the physicochemical properties of the materials and hence their catalytic activity. In this work, Cu/CeO_2 catalyst for carbon monoxide (CO) oxidation was synthesized by four different methods which are impregnation (Cu/CeO_2-IM), coprecipitation (Cu/CeO_2-CP), sol-gel (Cu/CeO_2-SG), and solution combustion synthesis (Cu/CeO_2-COM) to investigate the structure-activity relationship. The as-prepared catalysts were characterized by SEM-EDX, XRD, XPS, TEM and BET. Surface area measurements showed that area of catalysts ranges from 43 m^2/g to 104 m^2/g where (Cu/CeO_2-CP) exhibited the highest value. Furthermore, their catalytic performance towards CO oxidation was studied. Among them, Cu/CeO_2-COM. revealed the best performance where it afforded 100% CO conversion at 76 °C, which was attributed to the strong interaction between catalyst and support. The obtained data showed that Cu/CeO_2 catalyst can be used as substitute for noble-metal-based catalysts for low-temperature CO oxidation reaction.

IOT- SOLAR COLLECTOR-THERMO-ELECTRIC GENERATOR SYSTEM

Karim Ahmed,[1] **Zubair Ahmad,**[2] **Dong Suk Han,**[1,3]

[1]Centre For Advanced Materials (CAM), Qatar University, Doha, Qatar
[2]Young Scientists Center (YSC), Qatar University, Doha, Qatar
[3]Department of Chemical Engineering, College of Engineering, Qatar University, Doha, Qatar
E-mail: karim.ahmed@qu.edu.qa

The purpose of this study is to demonstrate a new design of a solar collector based on a conical concentrator and magnifier lens for application in a thermoelectric generator (TEG) system. The increased demand for green power production has led to the development of thermoelectric generator systems. A very promising alternative among other technologies is the TEG. This is a kind of energy conversion system that uses heat to generate electricity. The efficiency of thermoelectric energy is higher than other modes and they do not require moving parts, making them ideal for areas with no access to an electric grid. TEG is very simple, compact, cleaner, and renewable than other sources of energy, and as a result, it is an attractive choice for countries seeking to reduce their carbon footprint. The conical concentrator was designed with a concentration ratio of 2.25. The system consists of a 3D model of a conical concentrator covered with a reflective spray inside. It was developed by attaching a thermoelectric generator Peltier and a cooling heat sink to the bottom of the conical, a temperature sensor to the surface, and a magnifying lens to the top. In terms of dimensions, the magnifying lens and TEG Peltier measure 90 mm (diameter) and 40 mm × 40 mm × 4 mm, respectively. Two main processes are required for this design to work: collecting the heat from sunlight through a magnifying lens and then transferring it to one side of the TEG Peltier, while cooling down the other side of it by a cooling system. The temperature difference between these two sides allows for electricity production. The IoT part is used to monitor the temperature of the hot side of the Peltier besides the generated voltage. The temperature can be monitored by a sensor that connects to a microcontroller and transmits data to a web server. This study can contribute to providing accurate temperature and voltage readings, which will help determine if there is a problem with the solar collector.

LADANEIN-COATED IRON OXIDE NANOPARTICLES (γ-Fe_2O_3 NPs) AS A POTENTIAL ANTIVIRAL AGAINST CORONAVIRUSES

Seoyoung Lee,[1] Farah Benyettou,[1] Mourad Elhabiri,[2] Ali Trabolsi*[1]

[1]*Chemistry Department, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates*
[2]*Laboratoire d'Innovation Moléculaire et Applications (LIMA),CNRS-Unistra-UHA, European School of Chemistry, Polymers and Materials (ECPM),*
25, rue Becquerel, F-67087 Strasbourg, France
**E-mail:* ali.trabolsi@nyu.edu

Human coronaviruses (HCoVs) have been around for centuries and pathogenic coronaviruses such as severe acute respiratory syndrome (SARS) and the Middle East respiratory syndrome (MERS) have posed a major threat to global public health over the past two decades. As of March 17, 2022, there have been more than 400 million confirmed cases of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) and more than 6 million deaths due to the global pandemic. Despite the significant research effort, there is still no effective antiviral agent specifically targeting CoVs. The development of HCoV-specific antivirals is critical because the current strategy of testing existing broad-spectrum antiviral drugs against COVID-19 has shown them to be inefficient and have limited targeting, which can lead to serious side effects. In addition, there is a risk that new HCoVs (SARS-CoV-2 variants or new HCoVs) with severe symptoms will emerge in the future. For this purpose, ladanein-coated iron oxide (γ-Fe_2O_3) nanoparticles (NPs) are proposed as a promising solution. Ladanein is a 5,6,7-trihydroxy flavonoid with antiviral activity at the cellular entry-level of lipid-enveloped viruses, such as HCV or HIV, and strong antiviral activity against HCoV-229E has been recently discovered (collaboration with Karin Seron, CIIL, INSERM U1019, CNRS UMR9017, Lille, France). The coordination with the γ-Fe_2O_3 NPs is important as it can increase solubility and bioavailability, reduce toxicity, and control drug release through magnetic hyperthermia. Herein, ladanein-coated γ-Fe_2O_3 NPs (Lad-NPs) were successfully synthesized and characterized. The nature of interactions between ladanein and γ-Fe_2O_3 NPs and the concentration of each component were determined. The ladanein coating on NPs did not damage the NPs or change the morphology, size, and superparamagnetism of γ-Fe_2O_3 NPs. While free ladanein molecules were toxic to Hep G2 (liver) and HEK 293 (kidney) cells, Lad-NPs did not exhibit cytotoxicity, confirming their suitability as a drug. Cellular internalization of Lad-NPs was confirmed by fluorescence microscopy. The long-term goal is to test Lad-NPs on SARS-CoV-2 (COVID-19) and observe the effect of the γ-Fe_2O_3 NPs formulation on the antiviral activity of ladanein.

Lanthanide Tags in Search for Paramagnetically Induced Residual Dipolar Couplings in Small Molecules

Yara El Kazaz, Ali Yassin, Sally El Kantar, Elias Akoury

Department of Natural Sciences, School of Arts and Sciences, Lebanese American University, Beirut 1102-2801, Lebanon
Correspondence to elias.akoury@lau.edu.lb

Nuclear Magnetic Resonance (NMR) spectroscopy is an indispensable technique used in structure determination of small and macromolecules to study their physical properties and to elucidate characteristic interactions and thermodynamic processes. Quantum mechanics defines the theoretical description of NMR spectroscopy and treatment of the dynamics of nuclear spin systems. The phenomenon of Residual Dipolar Coupling (RDC) has become a routine tool for accurate structure determination by providing global orientation information of magnetic dipole-dipole interaction vectors within a common reference frame. This offers accessibility of distance-independent angular information and insights to local relaxation. The measurement of RDCs requires an anisotropic orientation medium for the molecules to partially align along the magnetic field. This can be achieved by introduction of liquid crystals or attaching a paramagnetic center containing a lanthanide ion. Although anisotropic paramagnetic tags continue to mark achievements in biomolecular NMR of large proteins, its application in small organic molecules remains limited. One challenge in the design of functional lanthanide-containing coordination compounds is the necessity for precise control of the Ln(III) inner coordination sphere due to varying degree of nondirectional bonding. Here, we propose a strategy for the synthesis of a lanthanide tag and the measurement of RDCs in organic molecules using paramagnetic lanthanide complexes.

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LEVERAGING DATA MINING FOR THE TEMPORAL AND GEOSPATIAL PREDICTION OF SHALE GAS WASTEWATER CHARACTERISTICS

Gasim Ibrahim,[1,2,3] Sunhwa Park,[1,3] Lucy Mar Camacho,[3,4] Debalina Sengupta,[2,3]
Nimir O. Elbashir,[1,3] Mahmoud M. El-Halwagi[2,3]
[1]*Chemical Engineering and Petroleum Engineering Program, Texas A&M University at Qatar, Doha, Qatar*
[2]*Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, USA*
[3]*TEES Gas & Fuels Research Center, College Station, USA*
[4] *Texas A&M University-Kingsville, Kingsville, TX, USA*
email: gasim.ibrahim@tamu.edu

The advent of hydraulic fracturing operations for the extraction of shale gas has led to a large boom in production across many regions of the globe. The hydraulic fracturing process utilizes and produces large quantities of water. The management of this water is a significant challenge due to the dynamic nature of shale gas waste water (SGWW), which varies significantly based on temporal and geospatial considerations. Significant research efforts have been put into developing treatment strategies for SGWW with the goal of reusing or recycling the water, instead of utilizing traditional disposal routes such as underground injection. However, the development of effective and efficient treatment strategies requires knowledge of the characteristics of the water to be treated, and obtaining the desired characteristics data can often be challenging. This makes a model-based approach for estimating the characteristics of SGWW appealing.

In this presentation we will highlight our efforts to utilize data mining techniques to develop a predictive model for the estimation of key SGWW characteristics in three major shale gas plays in the USA: Permian, Eagle Ford, and Marcellus. We collected sample data from publicly available data sources and consolidated them into one data set. We then conducted data pre-processing to reduce the variables in our data sets to the variables of interest, namely: sample age, well depth, sample location, TDS, and inorganic ions concentrations. The data was then classified based on shale play and sample TDS, and a final structured database was prepared. The data was then analyzed using standard statistical techniques. The analyses revealed large variance in SGWW characteristics between plays, and even within the same play. However, two relevant correlations were observed: a correlation between TDS and the various inorganic ions concentration in a sample, and a correlation between TDS and sample age. Regression analyses were then conducted to develop a model to predict a sample TDS based on sample age using a logarithmic formulation, and a model to predict the inorganic ion concentrations based on TDS concentration using a linear formulation. The models were then evaluated by calculating the median standard error between the model prediction and the actual values from data. The inorganic ions model gave reasonably accurately results for low and medium TDS samples, but displayed significant error for low TDS samples. The temporal model for TDS prediction gave fairly accurate results, but was limited to water originating from a single county in the Marcellus play due to limitations in the data. Additionally, we present two case studies to highlight how the model can predict the TDS and composition of SGWW with very limited information, such as the location and the age of a given well. This approach to quickly make reasonably accurate estimates for SGWW based on limited information will help stakeholders in the SGWW management process.

LOW-COST ELECTRODE FABRICATION FOR MICROBIAL FUEL CELL

Asif Saud, Hammadur Rahman Siddiqui, Syed Javaid Zaidi*
UNESCO Chair for Desalination and Water Treatment,
Center for Advanced Materials (CAM), Qatar University, Qatar
**E-mail address: szaidi@qu.edu.qa*

Abstract

Microbial fuel cells (MFCs) are now regarded as one of the primary sources of renewable energy [1]. Aside from that, the development of novel electrodes has always been a major priority in the production of green energy from MFCs. Many studies have been carried out using various types of electrodes, different mediums, and microbial colonies, and have been noted to impact the performance of MFCs. In this study, soil was employed as the substrate to illustrate the power production of a sediment microbial fuel cell (SMFC) developed with two distinct types of electrodes designed in laboratory settings. Recently, many researchers have been interested in the use of SMFCs in power generation.

In the current study, SMFC-1 was equipped with a stainless-steel electrode, whereas SMFC-2 was provided with a stainless-steel electrode covered with coal powder. According to electrochemical analysis, the SMFC-2 produced the highest voltage (830mV) and the maximum power (3129.1mW). X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FT-IR) analysis revealed that coal powder was well impregnated with stainless steel anode, and the chemical makeup of this electrode was identical to coal and stainless steel. As a result, we were able to successfully install the coal on stainless steel and acquire the intended results. The surface morphology of the electrodes was further evaluated using scanning electron microscopy (SEM) and atomic force microscopy (AFM), where it was discovered that bacterial accumulation was present, indicating a good deposition of bacterial biofilm. AFM results revealed a coarse surface that is favorable for bacterial growth due to increased surface area for bacteria accumulation. Furthermore, the X-ray photoelectron spectroscopy (XPS) results confirmed the elemental composition of stainless-steel electrodes with deposited coal powder on their surface.

Acknowledgements

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Reference

METHOD DEVELOPMENT FOR SELECTIVE AND NONTARGETED IDENTIFICATION OF NITRO COMPOUNDS IN DIESEL PARTICULATE MATTER

Mahmoud Bataineh

Department of Mathematics & Sciences, School of General Education, University of Doha for Science & Technology, Doha, Qatar

Nitro-aromatic compounds are associated with a host of adverse human health and ecological outcomes; however, current methods of detection are limited by the lack of accuracy for the nontargeted identification of nitro compounds. This paper describes the development of a novel, accurate, and selective method of identifying nitro compounds, especially nitro polycyclic aromatic hydrocarbons (PAHs), in complex soot mixtures. For the first time, high-performance liquid chromatography was used in combination with Orbitrap mass spectrometry for the nontargeted identification of nitro compounds. This method was validated on a mixture of 84 standard molecules containing 23 nitro compounds and then applied to a complex soot sample, the National Institute of Standards and Technology standard reference material (SRM) 1650a, to successfully identify 105 masses, 62% of which were monosubstituted nitro compounds. All nitro compounds reported in the latest certificate of analysis (COA) for SRM 1650b were successfully identified except for 1,3-dinitropyrene and 1,6-dinitropyrene. Compounds not reported in the COA of the SRM 1650b, including but not limited to 1,8-dinitropyrene, alkylated nitro-molecules of all masses in the COA of SRM 1650b, nitro-phenylnaphthalene isomers, dinitronaphthalene, nitro-phenols, nitro-keto-PAHs, nitro-carboxylic-PAHs, and other nitro partial polar compounds, were also tentatively identified. Future work will consider a larger set of classes, including isomers. This will help identify the chemical composition of mixtures in order to take proactive approaches to prevent health and environmental hazards.

Microwave Assisted Green Synthesis of Fe@Au core-shell NPs Magnetic to Enhance Olive oil Efficiency on Eradication of Helicobacter Pylori

poster

Najlaa S. Al-Radadi*

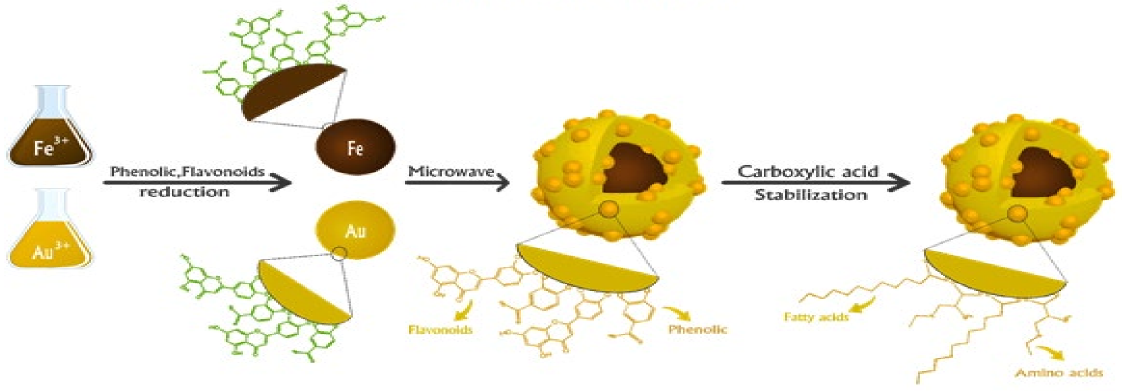
Department of Chemistry, Faculty of Science, Taibah University, P.O. Box 30002, Al-Madinah Al-Munawarah 14177, Saudi Arabia
E-mail address: nsa@taibahu.edu.sa Mobil: 00966505302644
https://orcid.org/0000-0003-3595-2231

Abstract

Eco friendly and green synthetic approach for the synthesis of metallic nanoparticles gained much importance in the recent era. In the present study, an environmental friendly and plant mediated synthetic approach was used for the synthesis of gold coated iron (Fe@Au) nanoparticles using extract solution of olive oil, licorice root *(Glycyrrhiza glabra)* and coconut oil (OLC). These extracts were acted as a reducing agent during the formation of core–shell nanoparticles that provides long-time stability, lower toxicity and higher permeability to specific target cells. In order to achieve the small sized, regular spherical shaped, and homogeneous nanoparticles optimum conditions were ensured. In fact, the use of microwave irradiation was offered higher reaction rate and better product. The Fe@AuNPs have been characterized by UV–Visible spectroscopy, Energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), High resolution Transmission electron microscope (HR-TEM), Fourier Transform Infrared Spectroscopy (FT-IR), high-performance liquid chromatography (HPLC), High angle annular dark-field scanning transmission electron microscopy (HAADF-STEM), Particle-Size Distribution (PSD), and Magnetic hysteresis loops. The synthesized gold coated iron nanoparticles showed significant antioxidant potential with maximum inhibition rates, the biosynthesized nanoparticles were also found effective against *Helicobacter pylori* (*H. pylori*) and ulcer.

Keywords: Fe@AuNPs, Antibiotics, Vitamin E, lauric acid, Anti-ulcer, *Helicobacter pylori*.

GRAPHICAL ABSACT



MIXED-LIGAND METAL COMPLEXES OF 4-METHYLBENZOIC ACID AND 2-METHYLIMIDAZOLE: SYNTHESIS, CHARACTERIZATION AND MICROBICIDAL ACTIVITY EVALUATION

Hassan K. Busari,[1,3] Sheriff O. Ayinla,[2,3] Ginikachukwu G. Nnabuike,[3], Misitura Lawal[4], Abdullah O. Rajee[3], Joshua A. Obaleye[3], Emmanuel A. Osuolale[3]

[1]*Department of Pure & Applied Chemistry, Osun State University, P.M.B 4494, Osogbo, Osun State, Nigeria*

[2]*Department of Chemical & Geological Sciences, Faculty of Natural & Applied Sciences, Al-Hikmah University, P.M.B 1601, Ilorin, Kwara State, Nigeria*

[3]*Department of Chemistry, Faculty of Physical Sciences, University of Ilorin, P.M.B 1515, Ilorin, Kwara State, Nigeria*

[4]*Department of Pure & Applied Chemistry, Kebbi State University of science and Technology, P.M.B 1144, Aliero, Kebbi State, Nigeria*

E-mail: hassan.busari@uniosun.edu.ng

Abstract

Two complexes [Cu(mba)$_2$(mim)(H$_2$O)(Cl)]-**T$_1$** and [Zn(mba)$_2$(mim)(H$_2$O)(Cl)]-**T$_2$** were synthesized by the reaction of their respective metal (II)chlorides with 4-methylbenzoic acid(mba) and a nitrogen donor heterocyclic ligand 2-methylimidazole(mim) in water, by stirring at room temperature for 3h.

The complexes were characterized by Fourier transform infrared radiation spectroscopy (FTIR), Powdered X-ray diffraction (PXRD), elemental analysis, molar conductance and melting point determination.

The FTIR results revealed bidentate and monodentate coordination modes respectively for 4-methylbenzoic acid and 2-methylimidazole in both complexes. The molar conductance of the complexes suggested their non-electrolytic nature in DMSO solvent. The PXRD analysis showed that **T$_1$** possess cubic system (a=20.1619A^o) while **T$_2$** possess orthorhombic crystal system (a=8.1953A^o, b=7.5577A^o, c=13.4593A^o). The two complexes are found to have trigonal bipyramidal geometry with two monodentate 4-methylbenzoic acid ligands, a monodentate 2-methylimidazole ligand, one aqua ligand and one chlorine ligand. The potential antimicrobial activity of the complexes and the ligands were investigated on some isolated pathogenic microbes: *Escherichia coli*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Aspergillus niger*, *Aspergillus flavus and Candida albicans* using agar diffusion method.

Both complexes showed better antimicrobial activities against some strains as compared to each parent ligand.

MOLECULAR MODELLING AND SYNTHESIS OF SMALL MOLECULE VIRAL INHIBITORS FOR SARS-COV 2

Khaya T. Gould,[1] **Willem A.L. van Otterlo**,[1] **Stephen C. Pelly**[2]

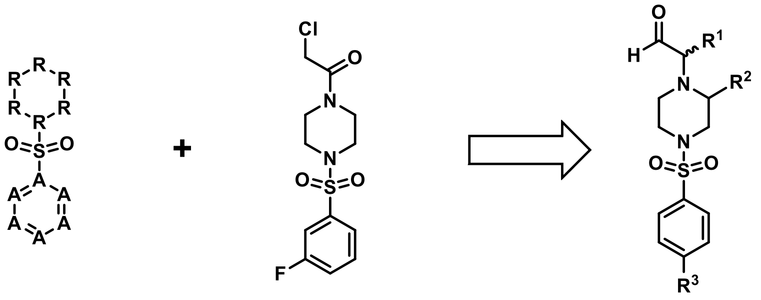
[1]*Chemistry and Polymer Science Department, Stellenbosch University, South Africa, 7600*

[2]*Chemistry Department, University of Emory, Atlanta, GA, USA, 30322*

E-mail: kgould@sun.ac.za

SARS-CoV 2 is a highly infectious virus responsible for the deaths of 6.05 million people worldwide and continues to spread. The 3 chymotrypsin-like proteases (3CLPro), the main protease of SARS-CoV 2, offers an ideal target for small molecule viral inhibition. Small-molecule sulfone-containing irreversible protease inhibitors, utilizing aldehyde electrophilic warheads, have been explored *in-silico* (PDB IDs: 6M0K, 7BUY, 5REK, and 5REF) in order to find new motifs that can be utilized as drug candidates. At present, three potential libraries have been generated using molecular modelling, focusing on modifications of the R^1, R^2, and R^3 positions (Figure 1).

Modifications to the R^1, R^2, and R^3 positions (Figure 1) were proposed to target the main protease binding site, involving Cys145 and His41 as key subunits for interactions in the binding pocket. In addition, the aryl-sulfonyl sub-structures were chosen due to their essential interactions with residues Glu166, Leu167, Pro168, and Gln192 within the binding pocket. So far, 18 compounds have been successfully synthesised for biological testing. Synthesis involving the R^3 position has progressed rapidly with the assistance of the high-yielding Suzuki-Miyaura reactions, offering upwards of 80% yield per reaction. This allowed for the fast and easy generation of a diverse library, limited only by our access to suitable boronic acids. Microwave-assisted Suzuki-Miyaura reactions on this scaffold have since proved successful, resulting in significantly reduced synthesis times.



2
Lu *et al.*[1] compounds with low micromolar IC_{50}s

3
Douangamath *et al.*[2] ligand from structure 5REK

4
General structure for libraries: R^1 based on different amino acids, R^2 on commercially available substituted piperazines, and R^3 on available substituted phenylsulfonyl chlorides

Figure 1: Figure to show the design and modification of the drug, bound in crystal structure 5REK.

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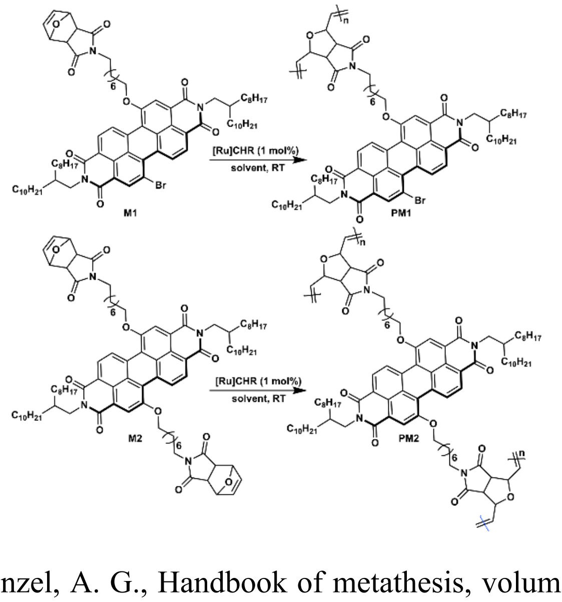
MOLECULAR-WEIGHT CONTROLLED METATHESIS POLYMERIZATION OF NORBORNENES CONTAINING *BAY*-FUNCTIONAL PERYLENE DIIMIDES

Santhosh Kumar Podiyanachari,[1] Maciej Barłóg,[1] Marc Comí,[1] Salahuddin Attar,[1]
Saeed Al-Meer,[2] Mohammed Al-Hashimi,[1] and Hassan S. Bazzi[1,3]

[1]*Department of Chemistry, Texas A&M University at Qatar, P.O. Box 23874, Doha, Qatar*
[2]*Central Laboratory Unit, Qatar University, P.O. Box 2713, Doha, Qatar*
[3]*Department of Materials Science & Engineering, Texas A&M University,*
209 Reed MacDonald Building, College Station, TX 77843-3003, United States
E-mail: s.podiyanachari@qatar.tamu.edu

Ring-opening metathesis polymerization[1] (ROMP)-derived mono-alkoxy poly(oxanorbornene imide) **PM1** and 1,7-di-alkoxy **PM2** bearing *bay*-functionalized perylene diimides (PDIs) were synthesized using ruthenium-alkylidene metathesis initiators. The monoalkoxy-derived PDI-based non-ladderphane polymer **PM1** displayed 67 to 77% of the *trans* olefin content in the polymer chain depending on the initiator used for the polymerization. In the case of the symmetrical 1,7-dialkoxy-derived PDI-based polymer **PM2** having the ladderphane type-structure, showed a significant amount of *cis* and *trans* olefin contents in the polymer chains, irrespective of the type of initiators used for the polymerization. ROMP of both monomers **M1** and **M2** proceeded in a well-controlled manner with a linear dependence of molecular weight on the monomer/initiator ratio. Optical properties of the ladderphane-based **PM2** and non-ladderphane-based **PM1** were characterized in both solution and the film state. X-ray diffraction (XRD) analysis for all the polymers showed significant π-stacking in the thin film state and the film morphology examined by AFM elucidated homogenous smooth polymer surface for both polymers in general, but with some irregularities observed for **PM1**.[2] Details of all these results will be presented.



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MULTIFUNCTIONAL POLYMERIC DOUBLE-LAYERED SMART COMPOSITE COATINGS FOR CORROSION PROTECTION OF STEEL

Norham Ismail, Ramazan Kahraman, Adbul Shakoor
Qatar University, Center for Advanced Materials
ni18647@qu.edu.qa

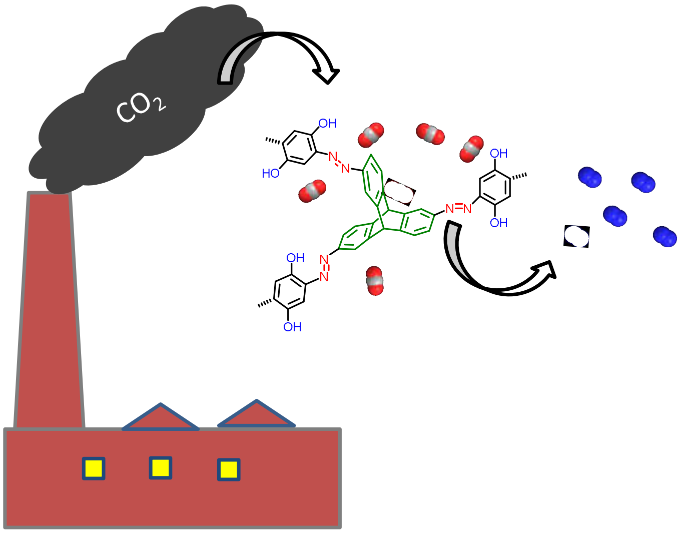
An epoxy coating modified with inhibitor and self-healing agent loaded to micro/nano reservoirs was developed for the smart corrosion protection of steel. To achieve this, an epoxy multilayered coating system containing a pre-layer composed of zinc-aluminum nitrate layered double hydroxide (Zn-Al/NO3 LDH) loaded with dodecylamine (DDA) used as an inhibitor (pH-sensitive) and a top layer (responsible for the self-healing effect) containing urea-formaldehyde microcapsules modified with linalyl acetate (LA) referred to as LMMCs. The Zn-Al/NO3 LDH and LMMCs were synthesized using the hydrothermal crystallization technique and in-situ polymerization method, respectively. The loaded Zn-Al/NO3 LDH (3 wt.%) and modified LMMCs (5 wt.%) were reinforced into an epoxy matrix to develop double-layer coating (DL COAT). For an exact comparison, a single-layer coating containing 3 wt.% loaded Zn-Al/NO3 LDH (SLDH COAT), single layer coating containing 5wt.% LA (LMCOAT) and blank epoxy coating (reference coating) were also developed. The developed epoxy coatings were characterized using XRD, XPS, BET, TGA, FTIR and EIS. SLDH COAT experiences a gradual increase in the global impedance with a significant decrease after 40 days of immersion in NaCl due to the absence of the healing effect. In comparison, the DLCOAT shows an incremental global impedance trend over the immersion time because of the self-healing agent and the inhibitor release that provides an excellent long-term barrier property with improved corrosion resistance.

NANOPOROUS POLYMERS WITH 3D-TRIPTYCENE FOR SELECTIVE AND EFFICIENT CAPTURE OF CARBON DIOXIDE

Mosim Ansari[1], and Neeladri Das[1]

[1]*Department of Chemistry Indian Institute of Technology Patna*
Bihta, India-801106
Author Email: mosim.pch16@iitp.ac.in

In the past few decades, global warming and its consequences have developed as serious environmental worry. Unrestrained growing concentration of carbon dioxide (CO_2) in atmosphere is regarded as one of the main culprits for global warming. Therefore, design of newer materials for efficient and selective uptake of CO_2 is of great importance. We have designed and synthesized several nanoporous polymers bearing 3D-triptycene in the polymeric network.[1-4] These polymers exhibited excellent thermal stability up to ($T_d > 380$ °C) and high surface area. The existence of nano porosity, π-rich cavities, and CO_2-philic groups in these polymers makes them effective adsorbent for capture of CO_2 (up to145 mg/g: 273 K, 1 bar) and H_2 uptake (up to 17.7 mg g^{-1} (77 K, 1 bar). These materials also have promising CO_2/N_2 selectivity values up to 84 at 273 K. Thus, these porous polymers can be considered as promising candidate in the domain of environmental remediation.



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Nature of the PES and Rate Determining Transition State in Associative CO_2 Insertion into the M-H Bond of *fac*-(bpy)$Re(CO)_3H$

Mariam Barakat[1], **Faraj Hasanayn***[1]

[1]*Department of Chemistry, American University of Beirut, Beirut 1107 2020, Lebanon*

E-mail: mab93@mail.aub.edu, fh19@aub.edu.lb

CO_2 insertion into the M-H bond of octahedral transition metal complexes yielding κ^1-metal-formate products is ubiquitous and routinely implicated in catalysis of reactions incorporating carbon dioxide hydrogenation. For many complexes, the reaction follows an associative mechanism that does not require opening an empty coordination site cis to the hydride on the metal. There have been, however, two views of the rate-determining step (RDS) in such non-classical mechanism: a linear hydride transfer transition state (TS) against a cyclic TS. CO_2 insertion into the Re-H bond of *fac*-(bpy)$Re(CO)_3H$ was previously reported to follow an associative mechanism in aprotic solvents and to exhibit substantially inverse deuterium kinetic isotope effects, KIE $\approx$ 0.55[1]. Herein we report a detailed DFT investigation of the associative (outer-sphere) potential energy surface (PES) into this system. We show that the PES can be divided into two stages. The first involves a low energy "linear" TS for bridging the carbonyl carbon and the intact metal hydride bond. The second is a subsequent stage that rearranges the bridged formate moiety via a higher energy cyclic transition state **TS$_{cyc}$** having an ion-pair character. The Gibbs free energy surface corresponds effectively to a concerted CO_2 insertion with the highest energy at **TS$_{cyc}$**. Consideration of **TS$_{cyc}$** as RDS affords computed activation free energies, solvent effects, substituent effects, and kinetic isotope effects that agree remarkably well with experimental data available for CO_2 insertion in this complex.

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New Approach to Modified the Chemical Structure of PVC and Enhancing It's Photo-Stability

Amer Adnan Hasan*, Mohammed H. Al-Mashhadani, Wedad H. Al-Dahhan, Emad Yousif

Department of Chemistry, College of Science, Al-Nahrain University, Baghdad, Iraq

*E-mail: amiadnan22@gmail.com

Abstract

Poly(vinyl chloride) was modified to develop an alternative support for the preparation of polymer-supported to enhance its photo-stabilizer. Commercially available poly(vinyl chloride) was synthetically modified to a polymer containing aromatic Schiff bases moieties. Firstly, the PVC polymer was reacted with ethylene diamine from one side using extra more equivalent of ethylene diamine to increase the probability of preventing cross-linking by two sides reaction. In the second step the corresponding aldehydes was reacted with amino group to make the Schiff base new molecules. Different techniques were used to demonstrate the chemical structure of synthesized materials such as FTIR, ^{1}H NMR, ^{13}C NMR, FESEM, EDX and TGA. Using above techniques it was confirmed the chemical structure and purity of synthesized materials.

In this work, these materials have been used as photo-stabilizers of PVC to reduce the photo-degradation of its polymeric chains. Many approaches were exhibited to evaluate the efficiency of modified PVC as photo-stabilizers such as FTIR, UV, weight loss, gel content, viscosity average molecular weight, light microscope, atomic force microscope, field emission scanning electron microscopy, and energy dispersive X-Ray (EDX) mapping. These studies were in agreement and demonstrated that new modified Schiff base polymers have excellent photo-stabilizers in comparison to blank PVC. Thus, they reduce the photo-degradation of PVC films compare to blank PVC after irradiation for 300 hours by UV light at wavelength 313 nm. This is because the attached units have highly conjugation system, which absorb light at UV region. The outcomes have been got in this study is significantly important to decrease the consumption of PVC around the world which is causing huge threaten to the environment especially the marine eco-system.

New Eco-Friendly Phosphorus Organic Polymers as Gas Storage Media

Dina S. Ahmed

Department of Medical Instrumentation Engineering, Al-Mansour University College, Baghdad, Iraq

* *Correspondence: dinasaadi86@gmail.com; dina.saadi@muc.edu.iq*

Abstract: Three phosphate esters were successfully synthesized from the reaction of 2-, 3- and 4-hydroxybenzaldehyde with phosphoryl chloride. Reactions of phosphate esters with benzidine in the presence of glacial acetic acid gave the corresponding novel phosphorus organic polymers containing the azomethane linkage. The structures of the synthesized compounds were confirmed by Fourier transform infrared spectroscopy, nuclear magnetic resonance and elemental analysis. Interesting physiochemical properties for the polymeric materials were observed using a combination of several techniques such as gel permeation chromatography, scanning electron microscopy, Brunauer–Emmett–Teller and nitrogen adsorption–desorption isotherm, Barrett–Joyner–Halenda and H-sorb 2600 analyzer. The mesoporous polymers exhibit tunable porosity with Brunauer–Emmett–Teller surface area (SABET = 24.8–30 $m^2.g^{-1}$), pore volume (0.03–0.05 $cm^3.g^{-1}$) and narrow pore size distribution, in which the average pore size was 2.4–2.8 nm. The synthesized polymers were found to have high gas storage capacity and physico-chemical stability, particularly at a high pressure. At 323 K and 50 bars, the polymers have remarkable carbon dioxide uptake (up to 82.1 $cm^3.g^{-1}$) and a low hydrogen uptake (up to 7.4 $cm^3.g^{-1}$). The adsorption capacity of gasses for polymer 5 was found to be higher than other polymers.

Keywords: eco-friendly polymers; phosphorus polymers; gas storage; gas uptake; gas capture; Brunauer–Emmett–Teller surface area

NEW SUBSTITUTED FUSED COUMARINS: SYNTHESIS AND APPLICATIONS

Mohanad Shkoor and **Raghad Bayari**

Department of Chemistry and Earth Sciences, Qatar University, P.O. Box 2713, Doha, Qatar.

Email: mshkoor@qu.eu.qa

New protocols for the synthesis of substituted fused coumarins were investigated. The reaction of diethyl 1,3-acetonedicarboxylate with various substituted 2-hydroxybenzylidineindenediones afforded fluorenone-fused coumarins. Moreover, the reactions of 3-aminocrotonirile and ethyl 3-aminocrotonate with substituted salicylaldehydes provided various pyridine-fused coumarins. All the prepared compounds prepared in moderate to high yields. The new fused coumarins were characterized by spectroscopic methods.

Since coumarins are in general eco-friendly compounds, the new substituted coumarins were screened for their corrosion inhibition activities in efforts to prepare non-toxic and environmentally benign anti-corrosion inhibitors. Some of those coumarins showed moderated to good corrosion inhibition activities in various HCl concentrations. The substituent effect on the inhibition activity was studied and the results provided a plan for further structural modifications.

It is well established that substituted coumarin compounds are fluorescent and can serve as fluorescence turn-on chemo sensors for the detection of heavy metals. The new coumarins were also evaluated as turn-on chemo sensors for a range of heavy metals. Some of the prepared coumarins found to be effective sensors for different metals including Cu^{+2} and Zn^{+2}.

NOVEL PRODUCTION OF BIOPLASTIC FROM QATARI DATES CORE WASTE

Ahmed Nader[1], Abdelrahman El-Rewaly[1], Atia Mahmoud[1], Munther Kandah [2] and Mohannad AlJarah[2]

[1]Al-Shahaniyah preparatory & Secondary School for boys - Qatar

[2]Doha University of Science & Technology – Qatar

munther.kandah@udst.edu.qa

Bioplastics are types of plastics that can be made wholly or partially from renewable natural resources. Therefore, bioplastics are sustainable, largely biodegradable and biocompatible. In this research, a novel production of bioplastic based on Qatari dates waste prepared by blending food grade gelatin, glycerin, polyvinyl alcohol (PVA) and dates powder to achieve the desired chemical and mechanical stability to be used in food packaging. In this work, fixed amounts of gelatin, glycerin and PVA dissolved in distilled water, then mixed with different amounts of Qatari dates core powder (0, 0.25, 0.5, 1.0, 1.5, 2.0 and 3.0 wt%) using magnetic stirring. Bioplastic sheets prepared by solution casting technique in polycarbonate mold. Different characterization techniques such as water uptake, gel fraction, tensile strength and migration test are used to investigate the samples' suitability for food packaging (mechanical stability and safety to food contact). The obtained results for our bioplastic exhibit high water retention near to 280% at low addition of dates. Gel fraction and tensile strength results, possess higher values (92% and 102 kgf/cm^2, respectively) with rising molar ratio of dates to certain amount. At high dates addition (3%), the failure in mechanical and crosslinking stability was observed. In addition, biodegradability test showed weight loss with the burial time. The produced bioplastic considered safe to contact with food according to the migration test that was done by Arab Center for Engineering Studies (ACES). Such results enhance the potential feasibility of our bioplastic for food reserving and packaging applications.

OPTIMIZATION BASED-MODEL FOR LOW-CARBON HYDROGEN ECONOMY: A CASE STUDY OF QATAR

Yasir Ibrahim, Dhabia M. Al-Mohannadi *

Department of Chemical Engineering, Texas A&M University at Qatar, Education City, PO Box 23874, Doha, Qatar

*Corresponding Author's E-mail: dhabia.al-mohannadi@qatar.tamu.edu

Abstract

Hydrogen has been hailed to play a crucial role in ending the world's dependence on fossil fuels and aiding the transition to climate-neutral economics in the future. Nevertheless, hydrogen can be only exists combined with other elements in form of a chemical bond. Therefore, hydrogen extraction necessitates energy-intensive processes, thus, generating a significant amount of Carbon Dioxide emitted into the atmosphere. This work introduces a comprehensive and strategic framework for planning and designing the hydrogen supply chain network through the low-carbon hydrogen economy. The optimization-based model will incorporate the multi-criteria analysis for hydrogen transportation modes (e.g., liquid hydrogen, ammonia, and liquid organic hydrogen carrier) simultaneously. These multi-criteria (metrics) will include economic, environmental, and safety. The behind form incorporating the multi-criteria analysis is to generate a Pareto-optimal solution to capture the trade-off that exists between these addressed metrics. The problem statement was formulated as Mixed Integer Linear Program (MILP) to identify the optimum decisions related to production, storage, and transportation from a number of many possible hydrogen networks. Consequently, the framework will provide an effective and efficient solution to boost the low-carbon hydrogen economy through simultaneously production and delivery of hydrogen, assessing renewable energy utilization, and incorporating carbon capture, utilization, and storage. The applicability of the proposed model was tested through a case study that resembles the industrial economy of Qatar.

ORGANO-CLAY COMPOSITES OF INTERCALATED ANILINE DERIVATIVES AND THEIR IN-SITU SYNTHESIZED SCHIFF BASES: STRUCTURAL AND ELECTRICAL BEHAVIOR STUDY

Ali J. A. Al-Sarray[1], Israa M. Al-Mousawi[1], Taghreed H Al-Noor[2], Yousif Abu-Zaid[2]

[1]Chemistry Department, University of Baghdad, College of Science, Iraq.
[2]Chemistry Department, University of Baghdad, College of Education Ibn Al-Haithem, Iraq.
E-mail: albaghdady1993@gmail.com

Organo-clay composites of two aniline derivatives and their Schiff base derivatives with unique structural and electrical properties were prepared by a solid state reaction using local bentonite clay. The obtained clay was modified and activated beforehand [1], and then used to prepare the Schiff bases in a process consists two steps; intercalating the aniline derivatives into the interlayers of the modified clay by a solvent-free reaction to form the organo-clay composites of the aniline derivatives [2], while the second step includes introducing the aldehyde derivative to the prepared composites in order to in-situ syntheses Schiff base derivatives in the interlayers of the clay mineral by condensation reaction and forms organo-clay composites of Schiff base derivatives.

The prepared composites were characterized by FTIR spectroscopy before and after the intercalation in the range of 400-4000 cm^{-1}, then the samples were examined via using X-ray diffraction analysis which shows changes in the d-spacing of clay smectic layers because of the presence of intercalated organic molecules. The chemical compositions of modified clay and the prepared composites were studied using X-ray Fluorescence. However, the surface morphology of the prepared composites was investigated by using Atomic force spectroscopy and Scanning Electron Microscope. On the other hand, diffused reflectance UV-Vis spectrometer was to obtain the electronic spectra of the prepared materials.

Electrical properties of the prepared composites, such as electrical impedance, dielectric permittivities, electrical dispatching, and electrical conductivity, were within (100 Hz to 1 MHz) range of frequencies in different temperatures. The prepared composites exhibit unique electrical properties especially for intercalated Schiff base derivatives. In addition, according to the calculated activation energies and dielectric relaxation times for the prepared composites, there are different types of charge carriers that have been proposed for various regions in the electrical spectra.

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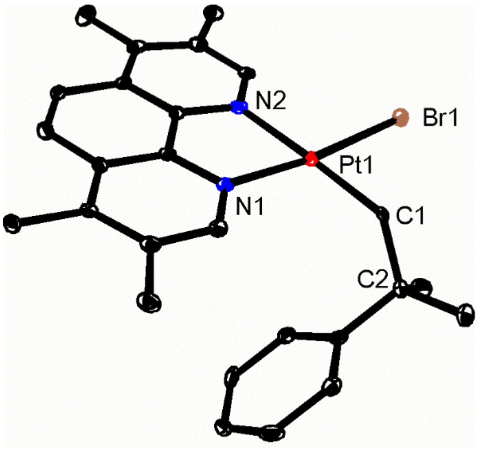
Oxidative Addition Of Halogens To A Dineophylplatinum(II) Complex: Halogen Complexes And Fluxional Platinum(IV) Complexes

Mohamed E. Moustafa, Mahmood Azizpoor Fard and Richard J. Puddephatt
Department of Chemistry, University of Western Ontario, London, N6A 5B7, Canada
E-mail: mmousta@uwo.ca

Many catalytic reactions involve oxidative addition and reductive elimination as key steps and so it is important to understand the reaction mechanisms and the resulting stereochemistry of these reactions [1-5]. Oxidative addition of halogens is one of the best known of these reactions, but this work will show that there are still subtle features to clarify. The reaction of a platinum(II) complex with a halogen usually occurs with *trans* stereochemistry to give the corresponding *trans*-dihalide derivative of platinum(IV)], though examples of *cis* oxidative addition are also known.

The reactions of [Pt(CH_2CMe_2Ph)$_2$(phen*)], **2**, phen* = 3,4,7,8-tetramethyl-1,10-phenanthroline, with halogens X_2 or their equivalents [$PhICl_2$ (as a Cl_2 equivalent), Br_2 and I_2] have been studied. The products [PtX(CH_2CMe_2Ph)(phen*)], **3**, and *cis,cis*-[PtX_2(CH_2CMe_2Ph)$_2$(phen*)], **4**, were formed in all cases. Remarkably, the octahedral platinum(IV) complexes **4** were fluxional in solution in CD_2Cl_2 or CD_3OD, as shown by their NMR spectra, and a mechanism involving very rapid reversible halide dissociation as a first step is established. The reaction of complex **2** in ether with $PhICl_2$ also gave an equilibrium mixture of three isomers of [PtCl(CH_2CMe_2Ph)($CH_2CMe_2C_6H_4$)(phen*)] by aromatic C-H bond activation. In other solvents, this reaction also gave [PtCl(CH_2CMe_2Ph)(phen*)] and then [PtCl_2($CH_2CMe_2C_6H_4$)(phen*)] and the C-H ond activation step is shown to occur at the axial site of the platinum(IV) center. The structures of eight complexes are established crystallographically.



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PERFORMANCE OF NICKEL-COPPER/ALUMINA CATALYTIC SYSTEMS IN DRY REFORMING OF METHANE: IMPACT OF COPPER LOADING AND SYNTHESIS TECHNIQUE

Omar El Hassan,[1,2] **Anjaneyulu Chatla,**[1] **Said Mansour,**[2] **Nimir Elbashir,**[1]

[1] Chemical Engineering Department, Texas A&M University at Qatar, Doha, Qatar
[2] Qatar Environment and Energy Research Institute, Doha, Qatar
Email: oalhassan@hbku.edu.qa

Dry reforming of methane (DRM) is a promising process that can convert carbon dioxide and methane, two of the most abundant greenhouse gases, into synthesis gas or syngas (a mixture of hydrogen and carbon monoxide). This vital chemical precursor can then be transformed into several value-added products, including ultra-clean fuels.

One of the main obstacles facing DRM is the rapid deactivation of economically desirable nickel-based catalysts due to carbon formation. Several studies investigated the different combinations of supports and promotors, which could improve the performance of nickel catalysts. However, a limited number of studies investigated the impact of varying synthesis techniques on the performance of the bimetallic catalysts for DRM. The current work aimed at studying the Ni-Cu/Al_2O_3 catalytic system in DRM, focusing on exploring the effect of copper loading on the catalyst characteristics and performance and the impact of the catalyst synthesis technique.

Three main preparation techniques were investigated, incipient wetness impregnation (IWI), co-precipitation (CP), and the sol-gel (SG) method. A comprehensive set of characterization techniques (ICP, BET, H_2-TPR, Chemisorption, XRD, XPS, SEM, TEM, EDS, TGA, TPO, DSC) was used to investigate crucial catalyst characteristics such as species reducibility, particle size distribution, crystallite diffraction patterns, and elemental composition.

The first part of the study is focused on the optimization of copper loading, catalysts synthesized by IWI only. It was found that medium copper loading (Ni: Cu=8:1) significantly improved catalyst performance compared to the monometallic variant and bimetallic catalysts with high and low copper loading. The formation of a Ni-Cu alloy reduced the amount of coke formed and increased catalyst stability. High copper loading (Ni:Cu=3:1) had an opposite effect as it reduced catalyst activity.

In the second part of the study,the monometallic and bimetallic catalysts (Ni:Cu=8:1) were synthesized using the SG and CP techniques. The bimetallic catalysts prepared by SG and CP were found to outperform their monometallic counterparts when tested for DRM. EDS analysis revealed that although the amount of copper introduced into the system aimed at creating a ‘medium’ loading, the synthesized catalyst had localized ‘high’ loading of copper encapsulating the active nickel sites in a core-shell shape. TGA of spent CP catalysts showed that the monometallic CP catalyst had a higher amount of carbon formed, indicating that the only logical reason for the underperformance of the bimetallic catalysts was copper segregation on the catalyst surface. The outcome of this study can be used to optimize the synthesis process of the bimetallic cataclys for DRM and other relations.

PHOSPHINE INCORPORATED METAL-ORGANIC-FRAMEWORK FOR PALLADIUM CATALYZED HECK REACTION IN BATCH AND FLOW CONDITIONS

Wenmiao Chen,[1] Insha Shaikh,[2] Fatma Ahmed,[2] Sahar Karkoub,[2] Sherzod T. Madrahimov,[3] Ma'moun Al-Rawashdeh[2]

[1]*Chemistry Department, Texas A&M University, College Station, TX 77843*
[2]*Chemical Engineering Department, Texas A&M University at Qatar, Doha, Qatar*
[3]*ScienceDepartment, Texas A&M University at Qatar, Doha, Qatar*

E-mail: cwm-tamu@tamu.edu
shaikh.ayaz@qatar.tamu.edu
fatma.ahmed@qatar.tamu.edu
sahar.karkoub@qatar.tamu.edu
sherzod.madrahimov@qatar.tamu.edu
mamoun.al-rawashdeh@qatar.tamu.edu

The development of recyclable catalysts used in chemical applications is a vital field of research, owing to the excessive use of harmful, non-recyclable materials in industrial processes contributing to environmental damage. The MOF (UiO-66) synthesized in this research has Zirconium-oxo clusters and BDC (terephthalic acid) which have the desirable characteristics required for its application in catalysis. In this work, we describe the application of MOF-immobilized Pd recyclable catalysts for Heck Coupling Reaction. We also established the generality of this reaction by running batch reactions on the substrate scope, that included 10 substituted aryl bromides with varying electronic properties. The catalyst synthesized, **UiO66-PPh$_2$-Pd**, was also applied for the coupling reactions under microflow conditions. **UiO66-PPh$_2$-Pd**, was analyzed by several characterization techniques including NMR, PXRD, TEM and SEM. The optimum conditions for Heck Coupling Reactions using **UiO66-PPh$_2$-Pd** as the catalyst was explored for batch conditions. Using the optimized conditions, various bromo-substituted substrates (0.2 mmol) were reacted with 0.3 mmol styrene for which a highest yield of 93% was obtained for 4-bromobenzaldehyde. Other substrates such as bromobenzene, 4-bromotoleune, 4-bromobenzonitrile, 4-bromoanisole, and 4-bromoaniline similarly had a high yield ranging from 90% to 92%. We also demonstrated that, the catalyst **UiO66-PPh$_2$-Pd**, can be recovered and reused for several catalytic runs. This research is vital to the understanding of the properties and applications of the synthesized MOF-catalyst **UiO66-PPh$_2$-Pd** and promoting the research in MOF based heterogeneous catalysts. This work further sheds light on the potential of the recyclable, efficient and robust catalyst, for the synthesis of value-added compounds and other industrial applications.

PHOTOCATALYTIC HYDROGEN GENERATION FROM SEAWATER USING HIGH PERFORMANCE POLYMERIC MATERIALS

Noora Al-Subaiei, [1] Ghalya Abdulla, [1] Dr. Mohammed Al-Hashimi, [2] Dr. Konstantinos E Kakosimos, [1]

[1]Chemical Engineering Department, Texas A&M University at Qatar, Doha, Qatar
[2]Chemistry Department, Texas A&M University at Qatar, Doha, Qatar
E-mail: noora.al-subaiei@qatar.tamu.edu, ghalya.abdulla@qatar.tamu.edu

Recently, there has been renewed interest in the use of solar energy as a resource to meet the world's energy needs in an environmentally sustainable way. Hence, our research focuses on the generation of hydrogen from non-fresh water using the sun as an energy source. The research aims to characterize, assess, and developed new research-grade materials and commercial photocatalysts that can achieve sunlight-driven unassisted photo-splitting of water.

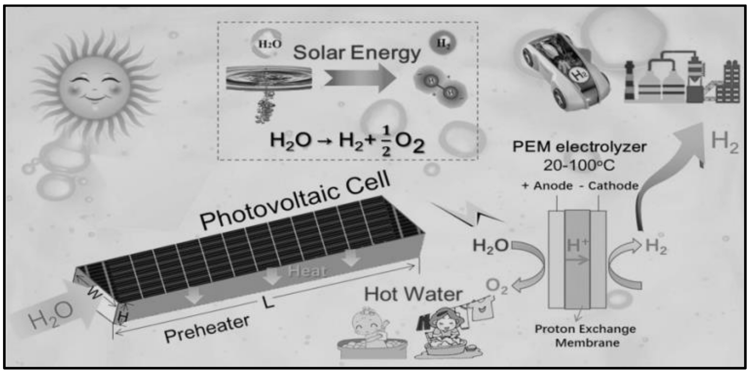

Figure.1 Image representing a combination of solar energy storage and water via hydrogen generation system. (Wang et al., 2019)

In this work, novel conjugated polymer nanoparticles were developed and characterized. The nanoparticles are composed of a donor-acceptor system where two acceptors, which were acceptor-1 (A1) and acceptor-2 (A2), were developed and tested, and different ratios of each donor-acceptor system were assessed. The use of platinum or molybdenum as co-catalysts was explored. Hydrogen evolution reactions with ascorbic acid as sacrificial reagent was performed using these materials and their performance was assessed.

The results show that the first system consisting of acceptor-1 and the donor (A1/D) produce more hydrogen than the (A2/D) system. Furthermore, the best ratio of donor: acceptor was determined to be 10:90 for the (A1/D) system. The use of platinum as a co-catalyst was shown to result in a better performance in terms of hydrogen production compared to the use of molybdenum. Furthermore, the results show that the use of nanoparticles suspended in solution results in a higher hydrogen evolution rate compared to the use of films. Hydrogen production of 2018 micromole per gram of catalyst per hour was achieved using the A1/D nanoparticle system with platinum.

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PHYTOCHEMICAL STUDIES ON THE FRUITS AND TWIGS OF *MAYTENUS DHOFARENSIS*

Fatma Al-Rubaiai, ZakiyaZ. Alshariqi, SafaAl-Haji, Majekodunmi O. Fatope, Syed I. Hassan, John Husband

Chemistry Department, Sultan Qaboos University, Muscat, Oman

Email: s87268@student.squ.edu.om

Different species of the genus *Maytenus* (*Celastraceae*) have long been used in traditional medicine for the treatment of cancer, gastric ulcers and arthritis. About 300 compounds have been isolated from the genus *Maytenus*, including triterpenes, lignans, flavonoids, and sesquiterpene pyridine alkaloids and some of them displayed antimicrobial, anti-protozoal, insecticidal, and cytotoxic activities [1].The present study investigates the natural products from the twigs and fruits of *Maytenus dhofarensis* that grows naturally in Dhofar, south-region of Oman. *M. dofarensis* is not a recognized medicinal plant in Omani herbal culture, but available ethnobotanical information showed that whenever goats eat the fruits, they fall ill with shivering attacks. Therefore, we speculate that the fruits of the plant might be cytotoxic or have cytotoxic compounds which can serve as anti-tumor or CNS active substances at controlled dosages! By discussing isolation methods, assay results and spectroscopic data, our work on the identification of the phytochemical components of selected extracts of the seed, seed capsule and twigs of the plant will be conveniently presented.

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POLYDOPAMINE COATED POLYETHERSULFONE MEMBRANE FOR THE TREATMENT OF HYDROCARBON CONTAMINATED WASTEWATER

Hamza Rekik[1], Shifa M.R. Shaikh[1], Mohamed K. Hassan[1]

[1]Center for Advanced Material, Qatar University, Doha, Qatar

Email: hamza.rekik@qu.edu.qa

In this study we try surface modification of a commercial polyether sulfone-based membrane to increase the durability of it. Membrane can be used for gas separation, water purification and desalination and last but not least, it can be used to decontaminate an area affected by an oil spill. In our case, we studied a flexible membrane to purify water polluted by oil. This type of membrane is still underdeveloped today compared to rigid membranes. Polydopamine is a material that can be applied to any surface in a simple way. In this study, we showed that a simple coating of polydopamine (PDA) on a commercial polyether sulfone (PES) membrane, which is a hydrophilic membrane, coupled with a ceramic membrane, could significantly increase the durability of the membrane while maintaining a percentage of organic pollutant removal of 95% to +/- 2%. If we compare the pristine membrane and the one with the PDA layer, we have noticed a decrease of the flux of more than 78% for the pristine one and an increase of the flux of 5% for the modified membrane with an elimination of 96% of the pollutants for both membranes after 5 cycles of 1 hour each one. These results are very promising in the field of flexible membrane purification.

POLYETHYLENEIMINE STABILIZED SILVER NANOPARTICLES AS AN EFFICIENT AND SELECTIVE COLORIMETRIC ASSAY FOR PROMETHAZINE

Daim Asif Raja,[1] **Muhammad Raza Shah,**[1] **Muhammad Imran Malik**[1,2,]*****

[1]H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences (ICCBS), University of Karachi, Karachi 75270, Pakistan

[2]Third World Center for Science and Technology, International Center for Chemical and Biological Sciences (ICCBS), University of Karachi, Karachi 75270, Pakistan

E-mail:*_mimran.malik@iccs.edu; m.imran.malik1@gmail.com_

Abstract

Metal nanoparticles (MNPs) possess distinctive properties, the surface electrons jumping from the valence band to the conduction band after interacting with electromagnetic radiation made them liable to have exceptional catalytic and optical properties. Due to this unique property, MNPs have been employed in a variety of applications such as catalysis, sensing, and drug delivery. Particularly metal nanoparticle-based colorimetric assays for drugs and pesticides are an emerging subject of current scientific research. Herein, polyethyleneimine (PEI) was used to stabilize silver nanoparticles (AgNPs) through a simple one-pot, two-phase protocol. As the main goal of the research, the synthesized PEI-AgNPs were employed for an efficient and selective quantitative detection of promethazine (PRO). The typical yellow color of PEI-AgNPs changed to orangish-brown as soon as PRO is added which is further endorsed by an increase in the intensity of the SPR band. The proposed sensor has proved to be efficient for quantitative detection of PRO in the presence of other interfering drugs and metal salts. The limit of detection, limit of quantification, and dynamic range of detection of PRO through PEI-AgNPs were found to be 0.003 µM, 0.008 µM, and 0.005-200 µM, respectively. Moreover, PEI-AgNPs allowed reliable, efficient, selective, and quick quantitative detection of PRO in real environmental, biological, and commercial drug samples. The proposed PRO sensor renders an excellent platform for its quick and on-spot determination without requiring a well-equipped lab setup. Up to the best of our knowledge, the proposed PRO sensor is first of its kind (colorimetric) in the list of proposed instrumental methods for determination of PRO.

Keywords: Polyethylenimine (PEI); Promethazine; PEI-AgNPs; colorimetric sensor; environmental samples, biological samples

POLYOLEFIN NANOCOMPOSITE COATINGS MODIFIED WITH ANTICORROSIVE PIGMENTS FOR THE CORROSION PROTECTION OF STEEL.

Muddasir Nawaz[1], Ramazan Kahraman[2,*], Maryna G. Taryba[3], Mohammad K Hassan[1], M. Attaei[3], M.F. Montemor[3], R. A. Shakoor[1,*]

[1] *1Center for Advanced Materials (CAM), Qatar University, 2713, Doha, Qatar*

2 Department of Chemical Engineering, Qatar University, 2713, Doha, Qatar

3 Centro de Química Estrutural, Institute of Molecular Sciences,

Departamento de Engenharia Química Instituto Superior Técnico,

Universidade de Lisboa, Av. Rovisco Pais 1049 001 Lisboa, Portugal.

E-mail: m.nawaz@qu.edu.qa

shakoor@qu.edu.qa

Corrosion-induced degradation phenomena are not only complex, but also cause economic losses and high operational and maintenance expenditures. Ceria nano particles loaded with 2-MBT were incorporated in Polyolefin coating to apply on steel substrate to study the corrosion protection and mechanical properties. For an exact comparison, non-modified polyolefin coatings, serving as reference were also prepared. The successful loading confirmed by Transmission election microscopy and Fourier transform infrared spectroscopy. While loading capacity of the Ceria nanoparticles was ~40 wt.% analyzed by Thermal gravimetric analysis and Brunauer–Emmett–Teller. Electrochemical impedance spectroscopy results show the improved and stable corrosion protection for modified coatings. The modified coatings significantly showed 95% better corrosion inhibition compared to reference coatings. The effect was attributed to the synergistic effect of the corrosion inhibition of cerium ions loaded 2-MBT and polyolefin healing capability. The mechanical properties of the coating were also improved which are confirmed by erosion and Vickers hardness testing.

Preparation, Structural Elucidation and Biological Potency of Some Novel Metal Drug Complexes

Joshua A. Obaleye[1]*, Abiodun A. Ajibola[1], Misitura Lawal [1], Hassan Busari[1], Mercy O.Bamigboye[2] and Ginikachukwu Nnabuike [1]

[1] Department of Chemistry,
University of Ilorin, Ilorin, Kwara State, Nigeria

[2]Department of Industrial Chemistry,
University of Ilorin, Ilorin, Kwara State, Nigeria

Corresponding Email : jobaleye@yahoo.com; jobaleye@unilorin.edu.ng

Abstract

Series of bioactive metal-drug complexes have been prepared using different synthetic techniques. The characterization of these new complexes were examined spectroscopically and by using FT-IR, UV-Vis Single crystal X-ray data were also used to reveal the structure of these complexes Some of the ligands used were anti-inflammatory, anti-tuberculosis, anti-cancer, antibiotics.

The inhibition of the growth of the bacterium, stopping or killing the microbes' infection is found to be mostly accompanied by the presence of a specific antimicrobial agent. There are many antibacterial and antifungal agents in the market that have been used till date. Though there are shortcomings on some of them which requires further improvement or a new discovery that can be more effective. Development of different anti-bacterial/fungal drugs has been supported by many sponsors with huge fund for several years. The development has also been limited by the persistence resistance arising from the different use of these antimicrobial agents.

With advances in medicinal discipline of chemistry, some novel complexes (metallodrugs) of *nd* transition metals with some Lewis bases containing nitrogen and carboxylate groups have been successfully synthesized and fully characterized. Apart from interesting structures displayed by these compounds, they were observed to be candidates for drug development due to their bioactive nature.

These compounds were characterized using spectroscopic techniques including HFEPR spectroscopy, microanalysis and single-crystal X-ray data. The *in vitro* antimicrobial activity of the investigated complexes against some fresh isolates of bacteria and fungi will be discussed.

PYRIDINE-IMINE METAL COMPLEXES IMMOBILIZED ON METAL ORGANIC FRAMEWORKS FOR HYDROSILYLATION OF OLEFINS

Beena Debnath, Vishmi Singhapura, Veeranna Yempally, Sherzod Madrahimov

Chemistry Department, Texas A&M University at Qatar, Doha, Qatar
Email:beena.debnath@qatar.tamu.edu

Metal-organic frameworks (MOFs) are gaining huge attention in the field of heterogeneous catalysis owing to their unique traits such as high crystallinity, large surface area, and easy separation of products from catalysts [1]. Hydrosilylation is a process used in industries to produce important silicon products. It is one of the most efficient methods for the formation of organosilicon compounds. It is mainly used in the silicon polymer industry to produce oils, rubber, and resins [2]. Several homogeneous catalysts based on Fe, Ni, Rh, Pt, and Rh [3] have been explored previously for efficient hydrosilylation of olefins. However, the separation of the products and recyclability of the catalyst hinder their application in industry. The superior catalytic activity of transition metal complexes immobilized on the MOFs compared to analogues homogeneous catalysts is well established [1]. Pyridine-imine metal complexes, specifically with Fe, exhibit excellent catalytic activity for hydrosilylation [4]. The present study aims to compare the catalytic activity of Fe, and Ni pyridine-imine metal complexes immobilized on UiO_66 NH2 MOF with respect to corresponding homogenous catalysts. Herein, we report the synthesis of Fe, and Ni pyridine-imine metal complexes immobilized on UiO_66 NH2 MOF. Characterization of catalysts are done with the help of XRD, TGA, and SEM-EDX analysis. In this study, we present the experimental observations of the hydrosilylation of olefins with Fe, and Ni pyridine-imine metal complexes immobilized on UiO_66 NH2 MOF as catalysts.

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Qatar Leadership Academy Plant Clinic and Research Center

Sunny Joseph
Qatar Leadership Academy
sjoseph@qf.org.qa

Most of us throw away a plant when it gets damaged or get some moth infections. And we replace it with another beautiful looking plant. We don't worry much when we come back after summer break to see our plants die due to lack of watering. We can always replace them. It has been our culture to worry much less about plants and their wellbeing. It doesn't matter if a plant doesn't reach its maturity, bear fruits and produce baby plants.

Plant Clinic and research center-A Mobile Plant Hospital to go to the fields to treat the plant diseases and injuries. Plant Clinic Idea-Originated from students of Agricultural Science Students and Gifted Program students of Qatar Leadership Academy. Our Mission: To provide accurate and timely plant disease diagnostic support to the agriculture/green industry and the people of Qatar to protect and secure our plant resources and to promote economic competitiveness. Our objectives: 1.Agricultural and herbal medicinal research, 2. Creating green spaces around Qatar, 3.Teaching and Producing plant doctors, 4. Conducting outreach programs and workshops for other schools and public.

In order to achieve our objectives, we have created or assembled the following resources. 1.Three industrial scale green houses and one herbal garden which are used as outdoor laboratories, 2.A high school diploma program called," Agricultural Science". This program is internally developed by science teachers of our school keeping the need of Qatar's sustainable development, 3.Knowledge and practice of variety of urban agricultural methods which could be used in limited spaces by people in cities who may not have a lot of space for farming or gardening.

Our project intends to educate the Qatari population and beyond about the importance of plants in our lives. We want people to understand that we rely on them for food, water, the air we breathe, our weather and climate and so on. We want people to learn about the plants and their need so that we can take care of them. QLA Plant clinic and research center came into being in an organic way. We needed outdoor laboratory meaning greenhouses, herbal gardens, green spaces, to complete many of our investigations. Our agricultural program has a human element in it. When we started learning about how plants communicate among themselves, how their needs are similar to humans, we started thinking about ways to stop the "use and throw" way of life. Most of the time, when people see plants go bad, they throw them away and plant new ones. Very rarely people nurse them back to health. Our respect for plants increases when we learn more about their medicinal uses.

We also intend to be plant doctors who may be able to conduct surgeries for plants. Who knows, one day we may be able to start a mobile hospital for plants by visiting the plants in their natural habitat and support their health. At QLA we show the respect to the plants that they deserve because we know we need them for a health life and sustainable world.

RESEARCH DATA MANAGEMENT FOR MATERIALS SCIENCE

Johanne Medina[1], Arif Shaon[2], Halima Bensmail[3], Fedwa El-Mellouhi[4]

[1] *College of Science and Engineering, Hamad Bin Khalifa University, Doha, Qatar*
[2] *Qatar National Library, Doha, Qatar*
[3] *Qatar Computing Research Institute, Hamad bin Khalifa University, Doha, Qatar*
[4] *Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha, Qatar*

Email: jmedina@hbku.edu.qa, felmellouhi@hbku.edu.qa

The need for good research data management practices is becoming more recognized as a critical part of research. This is driven by the exponential rate at which data is being generated from high-throughput computations in various disciplines including materials science, by different research groups and organizations. To maximize the use of this data, it is necessary to standardize, curate, preserve, and disseminate them in a way that is Findable, Accessible, Interoperable, and Reusable (FAIR) [1]. Developing a state-of-the-art data management system that adheres to the FAIR data principles, allows for effective and sustainable data preservation and re-use for the long-term. Doing so requires proper utilization of metadata which provide context (including provenance) to raw data and processes essential in materials discovery and validation [2]. This work aims to implement the best practices of research data management for materials science interdisciplinary teams by developing tools and methodologies to format and prepare data for sharing, storing, archiving and reuse. Best practices involve handling of data in a manner that meet all legal and confidentiality requirements while ensuring authenticity and integrity by implementing proper data formatting, version control, file naming, folder structures, and documentation strategies [3].

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RETROFITTING A NATURAL GAS AUTOTHERMAL REFORMING PLANT WITH CARGEN^{TM} TECHNOLOGY

Zeinab H. Ataya[1], **Mohamed Sufiyan Challiwala**[1,2,4], **Hanif Ahmed Choudhury**[1,4], **Debalina Sengupta**[2,4], **Mahmoud M. El-Halwagi**[2,4], **Elbashir, Nimir**[1,3,4]

[1]*Chemical Engineering Program, Texas A&M University at Qatar, PO Box 23874, Doha, Qatar*
[2]*Artie Mc ferrin Department of Chemical Engineering, Texas A&M University, TX, USA*
[3]*Petroleum Engineering Program, Texas A&M University at Qatar, PO Box 23874, Doha, Qatar*
[4]*TEES Gas & Fuels Research Centre (GFRC), College Station, TX, USA*
zeinab.ataya@qatar.tamu.edu

Reforming natural gas is an essential process in the gas-to-liquid (GTL) conversion to value-added chemicals. Decades of research and development have been put in developing and improving the commercialized reforming processes; autothermal reforming (ATR), steam reforming (SRM), and partial oxidation (POX). With the rapid increase in population and continuous industrial development, a global shift towards more environmentally friendly production processes is needed. Recently, dry reforming (DRM) received a lot of attention as an eco-friendly alternative for the conventional reforming processes. DRM has the potential to produce syngas while consuming CO_2 as a reactant. However, this process suffers from many downsides; coke formation, high CO_2 activation energy, and demand for continuous source of clean CO_2. Therefore, DRM could not yet be industrially implemented. Thus, the novel technology, CARGEN^{TM}, has been developed to address the DRM limitations. This technology is comprised of a two-reactor setup in which the first reactor converts CO_2 into high quality multi-walled carbon nanotubes (MWCNTs) while the second reactor produces syngas that meets the downstream processing requirements. Therefore, CARGEN^{TM} offers an opportunity to produce syngas at a low carbon footprint while also producing a valuable product, MWCNT, which significantly adds revenue to the GTL plant. In this work, a pre-existing GTL plant is retrofitted through replacing its conventional ATR unit with a CARGEN^{TM} unit to show the advantages of this novel technology. This was done by modelling ATR-based and CARGEN^{TM}-based GTL plants on ASPEN Plus® and comparing their key performance indicators; natural gas requirement, water generation, energy and power utilization. The simulation results show that while the CARGEN^{TM}-based plant consumes 61% more natural gas, it increases the water generation by 141% and reduces the oxygen requirement by 79%. Most importantly, it reduces the overall carbon footprint by 73% while producing 536 lb of MWCNT per barrel of GTL.

SELF-ASSEMBLY OF LANTHANIDE-DOPPED LANTHANUM HYDROXIDE VIA THE REACTION-DIFFUSION FRAMEWORK

Christina Katbe[1], Manal Ammar[1], Mazen Al-Ghoul[1], Louis A. Cuccia[2], Fiorenzo Vetrone[3], Adolfo Speghini[4]

[1]Department of Chemistry, American University of Beirut, Beirut, Lebanon
[2]Department of Chemistry and Biochemistry, Concordia University, Montreal, Canada
[3]Centre Énergie, Matériaux et Télécommunications, Institut National de la Recherche Scientifique, Université du Québec, Varennes (Montréal), Canada
[4]Nanomaterials Research Group, Department of Biotechnology, University of Verona, Strada Le Grazie 15, Verona, Italy
Email: crk16@mail.aub.edu

Nature's ability to self-organize has provided scientists with a huge spectrum of natural phenomena to investigate. In our work, we are particularly interested in the self-assembly of lanthanum hydroxide nanocrystals in a hydrogel matrix via a reaction-diffusion framework (RDF). The lanthanum hydroxide crystals are precipitated by pouring an outer electrolyte of concentrated ammonia onto agar gel containing lanthanum nitrate. Macroscopically, the resulting lanthanum hydroxide material forms Liesegang bands. SEM images of individual bands reveal a hierarchical structure of nano-platelets self-assembling into exquisitely shaped nano- and micro- spheres.[1] The mechanism of self-assembly is studied by coupling an electric field to a two-dimensional RDF. The effect of the field is noticeable as it enhanced the speed of the precipitation reaction front and accelerated the assembly of platelets to spheres, hinting at an underlying electrostatic mechanism controlling the self-assembly. We have also exploited this RDF system to develop a green, fast and easy preparation of Er^{3+} and Eu^{3+} doped La_2O_3 phosphors[2]. The lanthanide-doped La_2O_3 phosphors, obtained after calcination of the hydroxide, exhibit their classic emissions in the visible range, thus suggesting promising possibilities for light-emitting applications. Up conversion properties of the La_2O_3:Er^{3+} phosphors will be studied in due course.

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SILVER GRAFTED TI_3C_2-MXENE NANOCOMPOSITE AS NOVEL ANODE MATERIALS FOR LITHIUM-ION BATTERIES

Khadija Abdul Quddus[1], Hanan Abdurehman Tariq[2], Siham Yousuf Alqaradawi[1], Ramazan Kahraman[2], R. A. Shakoor[2]*

[1]*Department of Chemistry & Earth Sciences, College of Arts and Science, Qatar University, Doha, Qatar*

[2]*Center for Advanced Materials (CAM), Qatar University, Doha, Qatar*

Corresponding author: shakoor@qu.edu.qa

Ti_3C_2-Ag nanocomposites were synthesized, and their physical and electrochemical characteristics were investigated during the proposed study. This research aims at a new anode material for lithium-ion batteries (LIBs), Ag nanoparticle-decorated MXene (Ti_3C_2-Ag). The MXenes are resistant to oxidation, outstanding thermal and electrical conductivity, high electrochemical efficiency, composition flexibility, and a large specific surface area but because of the narrow gap between different MXene layers, coating the inner surface of MXene layers with metal oxide nanoparticles is difficult and time-consuming. SEM images revealed the growth of a nano-sized material with a well-homogeneous particle size distribution. Elemental mapping photos illustrate a uniform distribution of various elements throughout the material. The nanocomposite morphology developed consisted of Ag particles 50 nm in size, evenly dispersed in Ti_3C_2--MXene layers. For the electrochemical characteristics of Ti_3C_2--Ag nanocomposite, several electrochemical methods such as cyclic voltammetry, galvanostatic cycling, rates capability, and electrochemical impedance were comprehensively examined. When deployed as LIB anodes, Ti_3C_2--Ag nanocomposite outperformed pure Ti_3C_2-, providing greater performance and enhanced cycle efficiency. After 100 cycles at a current density of 0.1C, Ti_3C_2--Ag nanocomposite displayed good cyclic stability with a highly reversible potential of roughly 524 $mAhg^{-1}$. In addition, the rate capability is exceptional (up to 180 $mAhg^{-1}$ at a current density of 10C). These properties are obtained from the Ti_3C_2--Ag nanocomposite's unique composition. Furthermore, carefully coated Ti_3C_2- and Ti^{3+} layers produce high conductivity in MXene layers. Furthermore, Li+ ions can readily diffuse to the electrode through coated MXene layers.

SOLUTION COMBUSTION SYNTHESIS OF NICKEL-BASED MIXED TRANSITION METAL OXIDES FOR OXYGEN EVOLUTION REACTION IN ALKALINE MEDIUM

Aymen S. Abu Hatab,[1,2] **Yahia H. Ahmad**,[3] **Mohd. B. Abdul Rahman**,[1,2] **Siham Y. Al-Qaradawi**[3]

1. Department of Chemistry, Faculty of Science, Universiti Putra Malaysia UPM, 43400 Serdang, Selangor, Malaysia.

2. Integrated Chemical BioPhysics Research, Faculty of Science, Universiti Putra Malaysia UPM, 43400 Serdang, Selangor, Malaysia.

3. Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University, Doha 2713, Qatar.

E-mail: gs46963@student.upm.edu.my

In the last decades, the hydrogen production via water electrolysis has attracted scientists' attention. It is considered as one the most efficient technique which can produce a high purity CO_2-free hydrogen. However, the sluggish kinetics of oxygen evolution reaction (OER) remarkably increases the overpotential [1]. Nickel-based catalysts have been investigated extensively as powerful catalysts towards OER [2]. Inspired by this, we investigated the synthesis of nickel-based mixed transition metal oxides ($Ni_xM_{1-x}O_y$) and their catalytic performance towards OER. $Ni_xM_{1-x}O_y$ catalysts were synthesized by solution combustion synthesis (SCS) using the $Ni(NO_3)_2.6H_2O$, accompanied with smaller amounts of metal nitrates of Co, Fe, Mn, Cu or Cr, as oxidizer and glycine as fuel. Scanning electron microscope (SEM) micrographs confirms the porous structure for $Ni_xM_{1-x}O_y$, which is a common feature of combusted materials [3]. The EDX analysis confirms the composition of NiO and binary hybrid metal oxides. The morphology and particle size were measured by transition electron microscope (TEM). Spherical shapes were obtained for $Ni_xCo_{1-x}O_y$, $Ni_xMo_{1-x}O_y$, and $Ni_xCr_{1-x}O_y$ with an average particle size of 25.9 nm, 24.2 nm, and 29.0 nm, respectively, random agglomerates were obtained for $Ni_xFe_{1-x}O_y$ and $Ni_xCu_{1-x}O_y$, and flakes-like structure for $Ni_xMn_{1-x}O_y$. X-ray diffraction (XRD) of $Ni_xM_{1-x}O_y$ revealed well-defined diffraction peaks which confirms the crystalline nature of synthesized catalysts. The N_2-isotherms of $Ni_xM_{1-x}O_y$ were assigned to be type IV with H3 hysteresis, which is a characteristic feature for mesoporous materials. The electrocatalytic performance of the as-prepared materials was evaluated towards OER in 1M KOH solution. $Ni_xCo_{1-x}O_y$ exhibited the highest performance amongst other investigated electrocatalysts. For instance, it displays an overpotential of 339 mV at a current density of 1 mA cm^{-2}, onset potential of 1.605 V and a Tafel slope of 52.7 mV dec^{-1} in 1.0 M KOH solution. The superior activity of hybrid binary $Ni_xCo_{1-x}O_y$ is attributed to synergistic effect between Ni and cobalt, and the amount of Ni^{3+} and Co^{3+} on surface. It afforded the highest the Ni^{3+}/Ni^{2+} when compared to other electrocatalysts.

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Standard Methodology for Investigating Thermal Robustness of porous material

Satyanarayana Bonakala[1], Anas Abutaha[1], Elumalai Palani[1], Fadwa El-Mellouhi[1*]

[1]Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, P.O. BOX 34110, Doha, Qatar
Email: felmellouhi@hbku.edu.qa

Abstract

The development of robust and cost-effective methodology to discover (develop, design) an advanced porous functional material is of paramount importance to capture and sequester greenhouse gases. In this regard, we developed a hybrid methodology that consists of computational-led experiments then applied it to a reference metal-organic framework (MOF). We started with MOF structures as these materials are outclassed in gas adsorption/separation performance due to their flexibility in designing and functionality by applying reticular chemistry principles. Firstly, the structural model was obtained by performing electronic structure density functional theory calculations and the resultant MOF structure was validated by the experimental powder-X ray diffraction (PXRD). Further, thermal stability was delineated using force field-based MD simulations. We measure in-situ PXRD, thermogravimetric analysis, and differential scanning calorimetry to validate the theoretical outcomes. MOF structure shows thermal robustness until a temperature of 240 C at different atmospheric gases with a reversible breathing trend with temperature. The negative thermal expansion was also observed in the MOF structure as the tilting behavior of metal-ligand bonds while increasing the temperature. In addition, the adsorption isotherms and selectivity of CO_2 in CO_2/N_2 mixture were calculated using grand canonical Monte Carlo simulations. Our MOF structure shows a selective tendency towards CO_2 compared to N_2 gas which would be useful in the separation of CO_2 from flue gas mixture. The developed methodology can be expanded to refine the structure within the larger family of porous materials enabling considerable saving in spectroscopy resources to save time.

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STATE-OF-THE-ART PROCESS FOR HYDROGEN LIQUEFACTION INTEGRATED WITH LNG-BOG: ENERGY AND EXERGY ANALYSIS AND THE WAY FORWARD

Wisam alsaba[1], Saad A. Al-Sobhi[1], Mohammed Abdul Qyyum[2]

[1] Department of Chemical Engineering, College of Engineering, Qatar University, P. O. Box 2713, Doha, Qatar

[2] School of Chemical Engineering, Yeungnam University, Gyeongsan 712-749, Republic of Korea.

Email: wisam.alsaba@outlook.com

Abstract

Nowadays, the world-leading economies are shifting towards renewable energy sources to reduce carbon emissions and address climate change concerns. Hydrogen is regarded as a potential clean energy carrier that can replace conventional non-renewable energy sources. However, its low energy density makes its long-term storage and transportation over long distances unfeasible. Liquefaction is a promising solution to overcome these challenges. However, it is an energy-intensive process, and if hydrogen is the main energy provider, then 25-35% of its initial amount is consumed. To reduce this energy demand, LNG-BOG cold energy is utilized to liquefy the hydrogen. In the present study, a novel hydrogen liquefaction process based on the integration of LNG-BOG at the pre-cooling stage is proposed. The integrated process was simulated and analyzed using ASPEN HYSYS V11 simulator. The modified coordinate descent approach (MCDA) methodology was used to optimize the process and determine the optimal design variables. Based on the obtained results, the SEC of the proposed process was 7.65 kWh/kg$_{LH2}$, which is 45% lower than the base case. The exergy efficiency of the proposed process was 43.25%, which is 22% higher than that of the base case. The coefficient of performance and the figure of merit values for the proposed process were 0.287 and 0.432, respectively. The study is entailed to help practitioners in the field develop a future sustainable hydrogen economy, using adequate amounts of energy with minimized carbon emissions.

STRATEGIC CHEMICAL STRUCTURAL ENGINERRING IN THE DESIGN OF POLYMERIC SEMICONDUCTORS FOR OPTOELECTRONIC APPLICATIONS

Marc Comí,[1] Salahuddin Attar,[1] Maciej Barlóg,[1] Hassan S. Bazzi[1] and Mohammed Al-Hashimi

[1]*Department of Chemistry, Texas A&M University at Qatar, P.O. Box 23874, Doha, Qatar*

E-mail: marc.comi_bonachi@qatar.tamu.edu

The field of organic semiconductors has received in the last decade widespread attention from both academic and commercial perspective due to their rapid advances in high performance, flexibility, low cost and solution processability for the fabrication of optoelectronic devices in comparison with the inorganic counterparts based on silicon. It is well known that the intrinsic properties of semiconducting organic materials can be modified via chemical structural engineering during the design and synthesis of their monomers. This strategy based on alternation of conjugation with the accurate/proper electron-rich and electron-deficient units in order to adjust the highest occupied molecular orbital (HOMO) and the lowest occupied molecular orbital (LUMO) have become the major pathway to modulate optoelectronic properties such as the band gap. However, additional factors can influence the band gap of a semiconductor organic material such as, bond-length alternation, planarity, substituents effects, quinoid resonance, π-conjugation length, intra- and inter-molecular interactions, aggregation and crystallization, with clear effect in the device optimization.[1,2]

The four strategies evaluated: incorporation of side chains, exchange heterocycle moieties, photocyclization of aromatics and introduction of fluorine to enhance non-covalent interactions on the polymeric backbone have demonstrated to alter the physicochemical properties of the final materials. The optimization of these thermal, mechanical, optical, electrochemical and morphological properties of the polymer film led to an optimal selection of the optoelectronic application and an improvement on the device fabrication.[3,4]

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Structural Elucidation and Characterization of Cyclic–di–Nucleotides using NMR Spectroscopy

Christopher Saab, Bilal Nehmeh, Elias Akoury

Department of Natural Sciences, School of Arts and Sciences, Lebanese American University, Beirut 1102-2801, Lebanon
Correspondence to elias.akoury@lau.edu.lb

Cyclic dinucleotides are secondary signaling molecules, known in bacteria as intracellular secondary messengers, that act in response to an extracellular signal, the primary messenger. They are generated at the receptor of the cell surface to initiate downstream processes within the cell while prohibiting the first messenger of overcoming the cell membrane. In mammalians, these signaling molecules act as agonists of the innate immune response and regulate human genetic variations. Cyclic Adenonise Monophosphate (AMP) is a classical secondary messenger produced by the adenylate cyclase after activation of G-protein-coupled receptors. Similarly, cyclic-di-AMP are essentials in bacterial processes such as signal transduction in movement and production of viral factors. On the other hand, cyclic Guanosine–Adenosine Monophosphates (cGAMPs) bind and activate the endoplasmic reticulum surface receptor stimulator of interferon genes known as STING to produce interferons that trigger downstream immune responses to clear pathogenic threats.

Despite efforts in identifying interactions of cyclic dinucleotides with their corresponding protein binding partners for therapeutic intervention, the cellular cascades for regulation of the secondary messenger in viral bacteria and mammalian cells are not yet completely recognized. Using high-resolution Nuclear Magnetic Resonance (NMR) spectroscopy and a handful of physical-chemical methods, we shed lights on the structural characterization and chemical properties of different variants of cGAMP and c-di-AMP. We have identified the correct regiochemistry of the cyclic [G(2´-5´)pA(3´-5´)p] phosphodiester linkage and the connectivity of the primary amine group to the adenosine moiety. The complete structural elucidation of 2´3´ fluorescent GAMP, 2´3´ cyclic GAMP, 3´3´ cyclic GAMP and cyclic-di-AMP was accomplished from the chemical shift assignments of ^{1}H, ^{13}C, and ^{31}P resonances of nucleobases and ribose spin systems.

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Studying the efficiency of different functionalized PDMS coatings for high voltage application

Belal Salah[a], Fadi Z Kamand[a], Ahmed Abdelhay[a], Faozia Al-Shaibah[a], Sara Al-Abed[a], Mohammad K. Hassan [a], and Leena Al-Sulaiti[b].

[a] Center for Advanced Materials, Qatar University, P.O.Box 2713, Doha, Qatar

[b] Department of Math., Stat. and Physics, College of Arts and Sciences, Qatar University,
P.O.Box 2713, Doha, Qatar

Abstract: -

Improving the tracking and erosion reluctance of coated outdoor insulators using filled SIR (silicon rubber) of polydimethylsiloxane (PDMS) composites for high voltage insulation is a hot research topic specially for harsh environment locations. SIR-PDMS composites have unique physicochemical properties for high voltage insulation applications like chemical resistance, hydrophobicity with self-recovery, thermal stability, flame retardancy, and good mechanical properties. These properties are affected by the environment under aging in the field through exposure to direct sunlight, UV, Chrono, dry-band arcing, polluted rains, and industrial wastes which all lead to degradation and failure. Herein, we present the stability and efficiency of having different functional groups like Phenyl, and fluorine as terminated or branched groups of the PDMS matrix. Samples were tested for their tracking and erosion using the standard IPT test (@ 4.5KV). Furthermore, investigation and prediction of the degradation mechanism and the effect of the various functional groups on their physicochemical properties and stability will be also illustrated. Different techniques like Raman spectroscopy and FTIR (Fourier-transform infrared spectroscopy) were used to confirm the chemical structure. Surface morphology was studied using SEM (Scanning Electron Microscopy) and EDX (Energy Dispersive X-Ray) analysis. In addition, TGA (Thermogravimetric Analysis) was utilized to investigate the thermal stability of the coatings. This study will pave the way to use different functionalized chemical groups to enhance the thermal stability, increase the surface hydrophobicity with fast recovery for coatings surface under aging in the field and to increase the service life of commercial SIR composites coatings.

Sulfamethoxazole of Tri-Alkyltin(IV) Complexes as Photo-Stabilizers for PVC

Emad Yousif Al-Sarraj *, Emad Alhaydary

[1]Department of Chemistry, College of Science, Al-Nahrain University, Baghdad, Iraq

* Corresponding author. E-mail: emad_yousif@hotmail.com

Abstract

In this work, it was successfully synthesized new di- and tri-organotin(IV) complex Ph_3SnL, Bu_3SnL, and Me_2SnL_2 by reacting sulfamethoxazole drug as a ligand with different alkyl metal. The synthesized complex was fully characterized by fourier transform infrared, ^{1}proton nuclear magnetic resonance, ^{13}carbon nuclear magnetic resonance, ^{119}tin nuclear magnetic resonance and ultraviolet-visible spectroscopies. Field emission scanning electronic microscopy was also applied to study the surface morphology of synthesized complexes. Using above techniques it was confirmed the chemical structure and purity of synthesized materials. In this work, these materials have been used as photo-stabilizers of PVC to reduce the photo-degradation of its polymeric chains. Many approaches were exhibited to evaluate the efficiency of prepared organotin(IV) complexes as photo-stabilizers such as FTIR, UV, weight loss, gel content, viscosity average molecular weight, light microscope, atomic force microscope, field emission scanning electron microscopy, and energy dispersive X-Ray (EDX) mapping. These studies were in agreement and demonstrated that new complexes work as excellent photo-stabilizers of PVC. Thus they reduce the photo-degradation of PVC films containing these complexes compare to blank PVC after irradiation for 300 hours by UV light at wavelength 313 nm. It has also demonstrated that Ph_3SnL shows the best result as photo-stabilizer. This is because the complex has highly conjugation system by three phenyl groups compare to other complexes. The outcomes have been got in this study is significantly important to decrease the consumption of PVC around the world which is causing huge threaten to the environment especially the marine eco-system.

Keywords: Tri-alkyltin(IV) complex, Di-alkyltin(IV) complex, Sulfamethoxazole, Photo-stabilizers, PVC, blend films

SUPER OLEOPHILIC FIBER PACKINGS OF MESOPOROUS SILICA/TRI BLOCK COPOLYMER NANOCOMPOSITES FOR OIL WATER SEPARATION

Yara El-Gawady

Qatar University

yara.elgawady@qu.edu.qa

In this work we prepared inorganic mesoporous silica (MS) and add it in different concentrations (2, 4 & 7 wt.%) to Styrene-Isoprene-Styrene block copolymer (SIS) via electrospinning to produce an intact polymeric fibrous membrane, ultimately useful in selective oil absorption. The addition of MS to these fibers increased their diameters and created a swelled appearance as the MS concentration increases. The O/W separation efficiency is explored based on the oil absorption capacity of the samples as well as with the gravity driven oil filtration experiments. The best concentration for the SIS/MS composite is found to be at 4 wt.% MS, where the oil absorption capacity has increased by 150 % when compared to the neat SIS. Furthermore, we rolled the membrane into small similar cylindrical prototypes that were closely stacked in a funnel so that separated clean water is collected from the bottom of the funnel. The stability of the tubular packings through repeated absorption experiments and the absorption mechanism of the fiber are well addressed in this study.

Superior non-invasive glucose sensor using bimetallic CuNi nanospecies coated mesoporous carbon

A. Bahgat Radwan*^,1^, Sreedevi Paramparambath[2], John-John Cabibihan[3], Abdulaziz Khalid Al-Ali[3,4], Peter Kasak[5], R. A. Shakoor[1], Rayaz A. Malik[5], Said A. Mansour[6], Kishor Kumar Sadasivuni*^,1^

[a]Center for Advanced Materials (CAM), Qatar University, 2713 Doha, Qatar
[b]Department of Mechanical and Industrial Engineering, Qatar University, P.O. Box 2713, Doha, Qatar
[c]Department of Computer Engineering, Qatar University, P.O. Box 2713, Doha, Qatar
[d]KINDI Center for Computing Research, Qatar University, Doha, Qatar
[e]Weill Cornell Medicine-Qatar, Qatar Foundation-Education City, P.O. Box 24144, Doha, Qatar
[f]Qatar Energy and Environment Research Institute, Hamad bin Khalifa University, Qatar Foundation, 34110 Doha, Qatar

*Corresponding authors: **ahmedbahgat@qu.edu.qa** and **kishorkumars@qu.edu.qa**

Abstract

The assessment of blood glucose levels is necessary for the diagnosis and management of diabetes. The accurate quantification of serum or plasma glucose relies on enzymatic and nonenzymatic methods utilizing electrochemical biosensors. Current research efforts are focused on enhancing the non-invasive detection of glucose in sweat with accuracy, high sensitivity, and stability. In this work, nanostructured mesoporous carbon coupled with glucose oxidase (GO_x) increased the direct electron transfer to the electrode surface. A mixed alloy of CuNi nanoparticle-coated mesoporous carbon (CuNi-MC) was synthesized using a hydrothermal process followed by annealing at 700°C under the flow of argon gas. The prepared catalyst's crystal structure and morphology were explored using X-ray diffraction and high-resolution transmission electron microscopy. The electrocatalytic activity of the as-prepared catalyst was investigated using cyclic voltammetry (CV) and amperometry. The findings show an excellent response time of 4s and linear range detection from 0.005 to 0.45 mM with a high electrode sensitivity of 11.7 ±0.061 mA mM cm^{-2} in a selective medium.

SUPERIOR WATER FLUX OF SOLUTION BLOWN SPUN NANOFIBER-BASED THIN FILM COMPOSITE MEMBRANES FOR FORWARD OSMOSIS APPLICATION

Hammadur Rahman Siddiqui, Haleema Saleem, Syed Javaid Zaidi*
UNESCO Chair for Desalination and Water Treatment,
Center for Advanced Materials (CAM), Qatar University, Qatar
**E-mail address: szaidi@qu.edu.qa*

Abstract

Higher water flux, improved mechanical properties, low revere solute flux (RSF), and enhanced mechanical properties are the main requirements for effective membranes in desalination application, which would lead to decreased maintenance cost, improved energy efficiency, and operation easiness [1]. Among the different available technologies, forward osmosis (FO) is relatively energy efficient, when compared to other technologies, but have a very high RSF and low flux values. The main objective of this study to increase water flux while decreasing the RSF and enabling the membrane cleaning easier. The advanced and innovative solution blown spinning (SBS) process was used to develop nanofiber sheets, which has not been previously reported for application in membrane-based desalination. The study examines the performance of hot-press treated polysulfone (PSF) and polyether sulfone (PES)-based SBS nanofiber mat as the supporting layer of thin-film composite (TFC) membrane and graphene oxide (GO) incorporated polyamide (PA) layer as the selective layer for FO application.

Membrane performance was evaluated by carrying out FO testing with different feed and draw concentrations and various flowrates, and the results confirmed that extremely higher water flux and a minimal RSF values were achieved using solution blown spun nanofiber supported GO-TFC membranes. The membrane strength was examined by tensile testing, which confirmed an increase in mechanical strength up to four folds. Moreover, the contact angle analysis demonstrated the increased affinity of the developed membranes for water, and the AFM results confirmed the smooth texture of the prepared membranes, which is related to less fouling. The presence of GO and PA layers on the TFC was confirmed by FTIR analysis. Furthermore, the SEM micrographs indicated the solution blown spun fiber's highly interconnected fibrous structure and the successful formation of the PA layer.

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SUPPORTED IrNi NANOPARTICLES FOR GREEN HYDROGEN PRODUCTION BY PHOTOELECTROCHEMICAL WATER SPLITTING

Sifani Zavahir,[1] Umme Hafsa,[1,2] Dong Suk Han,[1,2]

[1]Center for Advanced Materials, Qatar University, P.O. Box 2713, Doha, Qatar
[2]Department of Chemical Engineering, Qatar University, P.O. Box 2713, Doha, Qatar
E-mail: dhan@qu.edu.qa

The world is transitioning to a hydrogen economy with a projected 12% market share in the energy sector by 2050 [1]. Hydrogen is mainly produced by methanol steam reforming (industrially) and electrochemical water splitting (in research scale). However, hydrogen produced by the photoelectrochemical (PEC) method means using fewer Pt catalysts is the most cost-effective and sustainable to address urgent energy concerns. Herein, we report a facile synthesis of uniformly distributed photoreactive iridium-nickel (IrNi) nanoparticles on a cost-effective activated carbon (AC) support with a low mass loading of 3 wt% for activity in electrochemical water splitting. Experimental results show that when the Ir:Ni ratio is properly regulated, hydrogen (HER) and oxygen evolution reaction (OER) can be induced under one sun (100 mW cm^{-2}) light irradiation at high rates over a wide pH range, compared to the intrinsic behaviors of individual Ir@Ac and Ni@AC. The material and electrochemical properties of the metal and alloy combinations affirm the cumulative effects of the relatively high crystallinity (among the materials in the study), the reduced charge recombination rate and the improved oxygen vacancies observed in the IrNi@AC electrode as reasons behind the superior PEC activity. The high level of durability can be seen in chronoamperometric studies that operated for 5 hours for HER and OER under light illumination. Overall water splitting examined in alkaline 0.1 M NaOH medium showed an overall cell voltage of 1.7 V at 10 mA cm^{-2} current density and 50 mV s^{-1} scan rate.

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SURFACE TUNING OF Pt-Pd CORE-SHELL NANOCUBES BY ELECTROCHEMICAL DEPOSITION OF Pt-Ru BIMETALLIC ALLOYS: A CATALYST FOR ENHANCED METHANOL OXIDATION IN FUEL CELLS

Ammar Bin Yousaf, Peter Kasak

Center for Advanced Materials, Qatar University, Doha 2713, Qatar
E-mail: ammar.chemist18@gmail.com (A. B. Y.), peter.kasak@qu.edu.qa (P. K.)

The methanol inlet fuelling is of great technological interest because of its potential application to direct methanol fuel cells (DMFCs) via electro-oxidation of methanol, which show significant potential as high-efficiency, low-emission future power sources. At present, significant efforts have been directed towards developing highly active catalysts for the electro-oxidation of methanol in DMFCs. Nanocomposite materials have been prepared by electrochemical fabrication of Pt-Ru bimetallic alloys on PdPt core-shell nanocubes. Electrochemical fabrication has done by using electrochemical chronoamperometric (CA) method for Pt-Ru co-deposition at constant potential of ca. 0.30V vs RHE. H_2PtCl_6 and $Ru(NO)(NO_3)_2$ are used as Pt and Ru precursor with 0.1M $HClO_4$ as electrolyte for the fabrication of Pt and Ru. The electrocatalytic activity as anode material for direct methanol fuel cells have measured by methanol oxidation reaction (MOR) activity in acidic medium. A significant improvement in the MOR activity is observed by increasing the atomic ratio of Pt in Pt-Ru bimetallic alloys co-deposition, while presence of Ru has no influence on chemisorptions of methanol but is significantly influenced the onset potential for MOR. Among all prepared catalysts, Pt_3Ru_1@PdPt-NCs and Pt_2Ru_1@PdPt-NCs have shown greater MOR activity than the commercial Pt/C (20%wt).

The results can be attributed to the collective effect of Pt-Ru bimetallic alloy nanoparticles and the enhanced electron transfer of core-shell PdPt-NCs in nanocomposite material. We have developed a facile, surfactant free and clean electrochemical fabrication method to develop good MOR active catalysts with better activity compared to that of commercial Pt/C catalyst. We have also focused and reduced the cost of catalyst by ultra low loading of Pt than the commercial catalyst by electrochemical fabrication method.

Acknowledgements

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SVMP INHIBITORS AS POTENTIAL ADAM8 INHIBITORS: AN IN SILICO STUDY

Hamda Aleissaee,[1] **Amie Jobe**[2], **Ranjit Vijayan**[2]

[1] *Department of Chemistry, College of Science, United Arab Emirates University, PO Box 15551, Al Ain, United Arab Emirates, E-mail: 201810405@uaeu.ac.ae*
[2] *Department of Biology, College of Science, United Arab Emirates University, PO Box 15551, Al Ain, United Arab Emirates*

ADAM8 is a member of the ADAM (a disintegrin and metalloproteases) family of membrane anchored proteases. Members of the ADAM family are implicated in various different diseases, however most documented is their role in cancer initiation and progression. Hence, identifying inhibitors to target ADAMs could assist in the development of therapeutic drugs. Interestingly, ADAMs were initially identified to be related to snake venom metalloproteinases (SVMPs). Specifically, SVMP P-III type possesses sequence similarities with ADAMs. The aim of this study was to explore if SVMP P-III inhibitors could inhibit ADAM8 through *in silico* methods including structural alignment, homology modelling, and molecular docking and molecular dynamics simulations. Identification of antivenom inhibitors for ADAM8 would aid in improving our understanding of the underlying mechanism as well as provide novel therapeutic drugs for the treatment of cancer.

SYMMETRIC CELL INVESTIGATION OF SODIUM VANADIUM FLUOROPHOSPHATE NASICON MATERIAL

Jeffin James Abraham[1], Ramazan Kahraman[2], Siham Al-Qaradawi[3], R. A. Shakoor[1,*].

[1]Center for Advanced Materials (CAM), Qatar University.
[2]Department of Chemical Engineering, College of Engineering, Qatar University
[3]Department of Chemistry & Earth Sciences, College of Arts and Science, Qatar University.
Email: jeffin.james@qu.edu.qa

The increasing demand for green energy is gaining substantial momentum during recent years. However, the shift from the conventional fossil fuel technologies to green energy is challenging due to lack of availability of suitable energy conversion and storage technologies. The current Li-ion battery technology aim to solve that issue. However, it still lacks in energy and power density suitable for the growing commercial needs. Moreover, since there is very few cost-effective Li recycling available currently, and Li reserves are limited, cost of batteries are high. Symmetric batteries are a potential solution to this cost problem arising in batteries, as the electrode material used in both the cathode and anode are same. Other salient features of symmetric ion batteries include reduced synthesis cost and effort, limited volume expansion in electrode materials, better safety and battery life, and reduced dendrite issues. The NASICON material $Na_3V_2(PO_4)_2F_3$ (NVPF) known for its large interstitial spaces and multi redox pairs of Vanadium at different voltages, make it suitable for use in symmetric cell configuration. Herein, we synthesize the phase pure NVPF material utilizing a simple sol-gel method and analyze it in a symmetric cell configuration. The working electrode potential range from 0 – 3.5 V for the symmetric cell, and a capacity of 85 mAh/g was achieved at 0.1C. Rate capability (RC) analysis of the symmetric showed electrochemical activity and stability up to 2C rate. Cycling analysis of the symmetric cells provided distinct results at both 0.1C rate and 1C rate. At 0.1C rate, a capacity retention of 92% is observed after 20 cycles, and at 1C rate, a capacity retention of 61% is observed after 1000 cycles. The symmetric cell underwent electrochemical characterization tests, such as, cyclic voltammetry (CV), galvanostatic intermittent titration technique (GITT), and Electrochemical Impedance spectroscopy (EIS) to understand ion diffusion behavior. Diffusion coefficients were calculated from CV, GITT, and EIS and was within the range of $\sim10^{-9}$-10^{-11} cm^2s^{-1} correlating with Na^+ diffusion in the symmetric cell. EIS analysis confirmed increasing bulk resistance, solid electrolyte interphase (SEI) resistance, and charge transfer resistance with number of cycles further explaining origin of capacity fade in the NVPF symmetric cell during cycling. Ex-situ analysis was conducted to understand the structure of NVPF at both the cathode and anode after 1000 cycles. A slight distortion in the cathode structure is observed which has caused capacity fade in the symmetric cell. However, there is no major structural damage observed in both the cathode and anode. The sodium vanadium fluorophosphate material, providing good electrochemical performance in a symmetric cell, can open new avenues towards developing long life and cost-effective batteries.

SYNTHESIS AND APPLICATION OF COBALT OXIDE (CO3O4)-IMPREGNATED OLIVE STONES BIOCHAR FOR THE REMOVAL OF RIFAMPICIN AND TIGECYCLINE: MULTIVARIATE CONTROLLED PERFORMANCE.

Ahmed S. El-Shafie [1], **Insharah Ahsan [1]**, Mohamed Radhwani [2], Mohammed Ali Al-Khangi [2]
and Marwa El-Azazy [1],*

[1] *Department of Chemistry and Earth Sciences, College of Arts and Sciences, Qatar University, Doha P.O. Box 2713, Qatar; aelshafie@qu.edu.qa (A.S.E.-S.); ia1803723@student.qu.edu.qa (I.A.)*
[2] *Al Jazeera Academy, Doha P.O. Box 22250, Qatar; 090055@aja.edu.qa (M.R.); asqtr74@gmail.com (M.A.A.-K.)*
***** *Correspondence: marwasaid@qu.edu.qa*

Cobalt oxide (Co_3O_4) nanoparticles supported on olive stone biochar (OSBC) was used as an efficient sorbent for rifampicin (RIFM) and tigecycline (TIGC) from wastewater. Thermal stabilities, morphologies, textures, and surface functionalities of two adsorbents; OSBC and Co-OSBC were compared. BET analysis indicated that Co-OSBC possesses a larger surface area (39.85 m^2/g) and higher pore-volume compared to the pristine OSBC. FT-IR analysis showed the presence of critical functional groups on the surface of both adsorbents. SEM and EDX analyses showed the presence of both meso- and macropores and confirmed the presence of Co_3O_4 nanoparticles on the adsorbent surface. Batch adsorption studies were controlled using a two-level full-factorial design (2^k-FFD). Adsorption efficiency of Co-OSBC was evaluated in terms of the % removal (%R) and the sorption capacity (q_e, mg/g) as a function of four variables: pH, adsorbent dose (AD), drug concentration, and contact time (CT). A %R of 95.18% and 75.48% could be achieved for RIFM and TIGC, respectively. Equilibrium studies revealed that Langmuir model perfectly fit the adsorption of RIFM compared to Freundlich model for TIGC. Maximum adsorption capacity (q_{max}) for RIFM and TIGC was 61.10 and 25.94 mg/g, respectively. Adsorption kinetics of both drugs could be best represented using the pseudo-second order (PSO) model.

SYNTHESIS AND ELECTROCHEMICAL PERFORMANCE OF $LiMn_2O_4$–MXene NANOCOMPOSITE CATHODES FOR HIGH-PERFORMANCE LITHIUM-ION BATTERIES

Muntaha Ali[1], Hanan Tariq[2], Zawar Alam Qureshi[2], R. A. Shakoor[2], Siham Alqaradawi[1 *]
[1]Department of Chemistry & Earth Sciences, College of Arts and Science, Qatar University,
P. O. Box 2713, Doha, Qatar
[2]Center for Advanced Materials (CAM), Qatar University, P. O. Box 2713, Doha, Qatar
E-mail: ma1804094@qu.edu.qa

Commercial lithium-ion batteries have employed expensive and toxic materials, causing in thermal runaway from overcharging or short-circuiting, which might result in a fire in the worst scenario. As a result, it's critical to develop new cost-effective cobalt-free cathode materials with higher energy storage capacity. Spinel lithium manganese oxide ($LiMn_2O_4$) is both economically and environmentally viable, in comparison to other lithium transition metal oxides. Moreover, $LiMn_2O_4$ has the potential to be a feasible cathode material for high-power lithium-ion batteries, due to its strong affinity for intercalating lithium ions, qualifying it to exhibit high energy density. However, the lower electronic conductivity of $LiMn_2O_4$ restricts its practical applications. MXenes are well acknowledged for their remarkable structural stability and high electronic conductivities; consequently, utilizing MXenes as a host material for $LiMn_2O_4$ could improve its structural and electrochemical properties. In the presented research, lithium manganese oxide ($LiMn_2O_4$) nanoparticles encrusted on MXene (Ti_3C_2) has been synthesized using microwave-assisted chemical coprecipitation technique. SEM analysis demonstrated that the in-situ method produced a homogeneous and conformal $LiMn_2O_4$ coating on the inner and outer layers of Ti_3C_2-MXene. The MXene-$LiMn_2O_4$ nanocomposite outperformed the pristine $LiMn_2O_4$ cathode electrochemically, exhibiting an electrochemical capacity of around 127 $mAhg^{-1}$ at 0.1C. MXenes function as a conductive matrix, providing an electrically conductive pathway for intercalating Li^+ ions. In conclusion, the introduction of MXenes to $LiMn_2O_4$ improves its electrochemical performance. The electrochemical analysis revealed that MXene-$LiMn_2O_4$ nanocomposites possess excellent electrochemical properties, indicating that MXene-based nanocomposites might be employed as cathodes in high-performance lithium-ion batteries.

SYNTHESIS OF NOVEL HETEROCYCLIC COMPOUNDS: ISOINDOLINONE, CINNOLINE AND BENZOTRIAZINE DERIVATIVES

Fatat B. El-Dhaibi, Makhluf J. Haddadin

Department of Chemistry, American University of Beirut, Riad El Solh, 1107 2020 Beirut, Lebanon
Email: haddadin@aub.edu.lb

Heterocyclic chemistry of organic compounds made an important progress in the last century. α-phentriazine, also known as benzo-fused analogs or 1,2,4-benzotriazine and cinnoline constitute an important class of the biological active compounds. Due to their wide range of applications in the biological, medicinal, pharmaceutical and therapeutic fields as well as their electronic and photonic properties, and despite all the monumental effort made to enhance the synthesis of these novels, a robust, economic and green synthetic methodology that increase the yield and generate a bulk amount of the desired product is urgently needed. Thus, we worked on developing and accessing an easy and time consumed process yielding our target products. The aim of our project is to synthesis a series of 1,2,4-benzotriazine derivatives and cinnoline compounds via the intermediate isoindolin-1-one. All previous studies confirmed the anticancer,[1, 2] antimalarial[3] and antifungal[4] activity of the 1,2,4-benzotriazine compounds.

Indeed, 27 compounds (isoindolinone, cinnoline and 1,2,4-benzotriazine) were synthesized in two steps reactions each. Whereby, after each step, all the structures of the stated compounds were isolated as yellow solid products, and characterized by spectroscopic analysis: FTIR, ^{1}H NMR, ^{13}C NMR, ^{13}C NMR DEPT 135, and melting points. The molecular weight was determined by high resolution mass spectroscopy (HR-MS). Moreover, the X-ray structure of the product: methyl 2-(7-methoxybenzo[e][1,2,4]triazin-3-yl)benzoate was resolved by Dr. James Fettinger and Distinguished Professor Mark Kurth, from the Chemistry Department of the University of California, Davis CA, USA.

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SYNTHESIS OF SILVER NANOPARTICLES ON ACTIVATED AND DEHYDRATED CARBON FOR ANTIBACTERIAL PROPERTY

Aisha Al Musharrafi,[1] Elsaid EL Shafey,[1]

[1] *Chemistry Department, Sultan Qaboos University, College of Science, Muscat, Sultanate of Oman*

s117827@student.squ.edu.om

Metallic nanoparticles have received interest over the past few years due to their potential impact in many areas of science. In particular, silver nanoparticles have garnered attention due to its unique physical, chemical and biological properties [1]. Silver nanoparticles exhibit high intrinsic antimicrobial activity that can be applied for medical purposes to reduce infection as well as eliminate bacteria [2].

Activated and dehydrated carbons were prepared from mandarin peel (*citrus reticulate*). Activated carbon was prepared using NaOH activation at 700 °C. AC was oxidized using nitric acid to produce oxidized activated carbon (OAC). Dehydrated carbon (DC) was prepared from MP at 180 °C using sulfuric acid (SDC) or phosphoric acid (PDC). Ag^+ ions were reduced to Ag^0 as nanoparticles (AgNPs) on carbon surfaces, as confirmed by SEM and x-ray diffraction. Cumulative silver loading was carried out for 3 successive cycles showed enhanced silver uptake of 630, 972, 755 and 589 mg/g on AC, OAC, SDC and PDC at 50 °C, respectively. Ag^0-loaded carbons were tested for antibacterial properties against *E. coli, S. aureus and P. aeruginosa* bacteria in terms of inhibition zone and growth inhibition. All Ag^0-loaded carbons showed effective antibacterial activities.

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SYNTHESIS, CHARACTERIZATION, BIOLOGICAL AND MOLECULAR DOCKING STUDIES OF OXAMIDE DERIVATIVES

Maira Naz, Uzma Ashiq, Rifat Ara Jamal, Naseema Perveen Malik

Department of Chemistry, University of Karachi, Karachi-75270, Pakistan

Email: uzma.ashiq@uok.edu.pk

The aim of this study is to synthesize and characterize a new class of oxamides and to study its biological significance. From the literature survey, it is investigated that this class of compound has significant biological application, but still insufficient information is available on biological studies of oxamides. Compounds of oxamides (**1-20**) were synthesized by reaction of aniline with oxalyl chloride. The structure of synthesized compounds was confirmed by ^{1}H-NMR, EI-MS, IR spectroscopy and X-ray diffraction studies. Additionally, computational approach was also applied to calculate vibrational frequencies of synthesized compounds and both techniques showed comparable result. ^{1}H-NMR was confirmed the *trans* conformation of compounds by giving the spectra of half protons because of plane of symmetry in structure. EI-MS predict the correct molecular mass of compound which was confirmed by CHN. Non- enzymatic (DPPH), enzymatic (lipoxygenase and xanthine oxidase) antioxidant activities and enzyme inhibition (α-glucosidase) studies of all synthesized compounds were performed. Oxamides exhibit promising antioxidant and enzyme inhibition activity. Most of the compounds showed significant antioxidant radical scavenging potential compared with the standard butylated hydroxyanisole (BHA). All compounds showed proficient inhibitory potential in different enzymatic assays. Out of 20 oxamide, (9) compounds exhibit good inhibitory potential (IC_{50} ranges between 38.2-75.8 μM) of α-glucosidase, when compared with the standard 1-deoxynojirimycine (DNJ) with IC_{50} = 425.6 ±1.3 μM. It is an enzyme which is related to glucose level in blood, the inhibitor of this enzyme can be used to cure diabetes type II. Further studies are still required to understand its pharmacological role to use oxamides in therapeutic drugs. Molecular docking studies were performed for the evaluation of binding mechanism of oxamide compounds in the pocket of α-glucosidase enzyme. Docking scores based on EADock score, inhibitory activities and docking energies showed similar trend of inhibition.

SYNTHESIS, STRUCTURAL CHARACTERIZATIONS, ANTIBACTERIAL STUDIES OF SOME TRANSITION METAL COMPLEXES OF SCHIFF BASE DERIVED FROM AZO AND P-VANILLIN

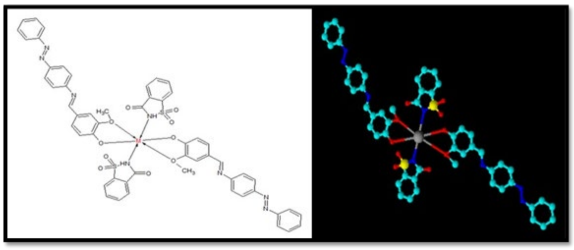
Salam R Al-Ayash[1], Taghreed H Al-Noor[1]

[1]Chemistry Department, University of Baghdad, Ibn -Al-Haithem College of Education for Pure Science, Iraq

salamriyadhr1251@gmail.com

In this work, Schiff base (LH) named 1- 2-methoxy-4-[(E)-({4-[(E)-phenyldiazenyl] phenyl} imino)methyl]phenol containing the azo group, was synthesized from the reaction of P-Aminoazobenzene with P-Vanillin. The mononuclear mixed ligand complexes of Copper(II), Nickel(II), Cobalt(II), Iron(II) and Manganese(II) complexes of the Schiff base with Saccharin-(Sac) ligand were prepared in the formula [M(L)$_2$(Sac)$_2$] and characterized using elemental analyses, FT-IR, UV-visible spectroscopy, magnetic susceptibility and conductance measurements: (^{1}H and ^{13}C) NMR and mass spectra of the ligand were also recorded (Figure:1). Through spectroscopic studies, we found that the metal ions coordinate with the (LH) ligand via oxygen atoms and the (Sac) ligand via nitrogen atom (Figure:2). The complexes prepared were used as dyes through their application in dyeing wool and cotton fabrics, and the fastness properties and color strength of the dyed fabric were evaluated and gave excellent results.

In addition, the ligands and complexes were evaluated for both their in vitro antibacterial activity using the disc diffusion method.

	
Figure 1: The structure of (LH)	Figure 2: The structure of the [M(L)$_2$(Sac)$_2$]complexes M=Cu(II), Ni(II), Co(II), Fe(II) and Mn(II)

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TEMPLATE-DIRECTED COPPER (II)-ORGANOPHOSPHONATE COMPOUNDS

Kanagaraj Rajendiran [1] **and Avijit Kumar Paul** [1]

[1]*Department of Chemistry, NIT-Kurukshetra, Haryana-136119, India.*

krajchemist@gmail.com; Mob: +91-[9840624203]

Although the silicate, phosphate, sulfate, thiosulfate, borate based open-frameworks are investigated intensively, [1-3] amine templated organophosphonate based framework structures are not studied so far. In our present study, three new open-framework compounds of copper organophosphonates have been synthesized by hydrothermal methods and their structures determined by single crystal X-ray diffraction studies. All the three compounds, [amine][Cu(Phosphonate)$_2$],**I**, [amine][Cu$_3$(Phosphonate)$_2$],**II** and [amine][Cu$_3$(Phosphonate].4H$_2$O, **III** possess molecular structure, one-dimensional ladder structure and two-dimensional layer structures connecting through the copper and diphosphonate units, and the protonated amine molecules are sitting inside the channel. The compound **II** shows an eight-membered ring and compound **III** contains four and eight-membered rings assembled through vertex-sharing {CuO$_4$}, edge-sharing {CuO$_5$} unit. The compounds are synthesized under the hydrothermal condition and characterized by powder XRD, IR, TGA. The various structural and physical properties will be discusses in detail.

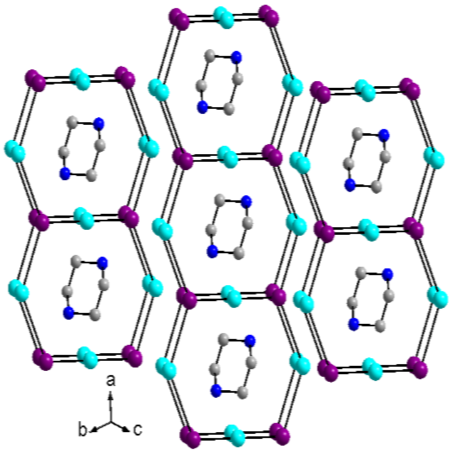

Fig1: Compoud II-1D-net structure

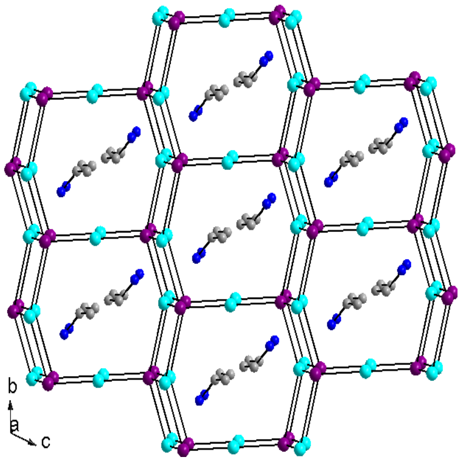

Fig2: Compound III-2D- net structure

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THE SEPARATION OF EMULSIFIED WATER/OIL MIXTURES THROUGH ADSORPTION ON PLASMA-TREATED POLYETHYLENE POWDER

Asma Abdulkareem[1], Patrik Sobolˇciak[1], Anton Popelka[1], Igor Krupa[1]

[1]*Center for Advanced Materials, Qatar University, P.O. Box 2713 Doha, Qatar*
E-mail: asma.alkareem@qu.edu.qa

This research work addresses the preparation and characterization of efficient adsorbents for tertiary treatment (oil content below 100 ppm) of oil/water emulsions. Powdered low-density polyethylene (LDPE) was modified by radio-frequency plasma discharge and then used as a medium for the treatment of emulsified diesel oil/water mixtures in the concentration range from 75 ppm to 200 ppm. Plasma treatment significantly increased the wettability of the LDPE powder, which resulted in enhanced sorption capability of the oil component from emulsions in comparison to untreated powder. Emulsions formed from distilled water and commercial diesel oil (DO) with concentrations below 200 ppm were used as a model of oily polluted water. The emulsions were prepared using ultrasonication without surfactant. The droplet size was directly proportional to sonication time and ranged from 135 nm to 185 nm. A sonication time of 20 min was found to be sufficient to prepare stable emulsions with an average droplet size of approximately 150 nm. The sorption tests were realized in a batch system. The effect of contact time and initial oil concentrations were studied under standard atmospheric conditions at a stirring speed of 340 rpm with an adsorbent particle size of 500 microns. The efficiency of the plasma-treated LDPE powder in oil removal was found to be dependent on the initial oil concentration. It decreased from 96.7% to 79.5% as the initial oil concentration increased from 75 ppm to 200 ppm. The amount of adsorbed oil increased with increasing contact time. The fastest adsorption was observed during the first 30 min of treatment. The adsorption kinetics for emulsified oils onto sorbent followed a pseudo-second-order kinetic model.

THE SYNTHESIS OF ISOCHROMANS FROM BIO-BASED ANACARDIC ACID DERIVED FROM CASHEW NUTSHELL LIQUID (CNSL)

Bianca Davids[1], Kennedy Ngwira[1], Charles de Koning[1]

[1]*Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa*
Email: bianca.davids@wits.ac.za

Huge quantities of waste materials find landfills as their final destination, especially in a time where environmental awareness has become critical as a means to address issues related to food security, health, industrial restructuring, and energy security. As a result, there has been a shift towards crafting new products and chemical building blocks derived from waste materials [1,2]. One example is cashew nutshell processing which has gained attention due to the valuable greenish-yellow viscous liquid inside the shell known as cashew nutshell liquid (CNSL).

Anacardic acid, the major component of natural CNSL, has gained much interest from scientists due to its biological activities, which include antitumor, antioxidant, gastro-protective, and antibiotic activity [3].

The synthesis of two racemic isochromans derived from bio-based anacardic acid obtained from cashew nutshell liquid (CNSL) is described. Two key steps for the synthesis of the isochromans were utilized. (i) The benzylic bromination of methyl 2-methoxy-6-pentadecylbenzoate was accomplished with *N*-bromosuccinimide in the green solvent *tert*-butyl acetate. (ii) Exposure of the two secondary alcohols 1-(2-methoxy-6-(prop-1-en-1-yl)phenyl)ethanol and 1-(2-methoxy-6-(pentadec-1-en-1-yl)phenyl)ethanol to potassium *tert*-butoxide resulted in the formation of the isochromans, *trans*-8-methoxy-1,3-dimethylisochroman **2** and *trans*-8-methoxy-1-methyl-2-tridecylisochroman **3** (Figure 1).

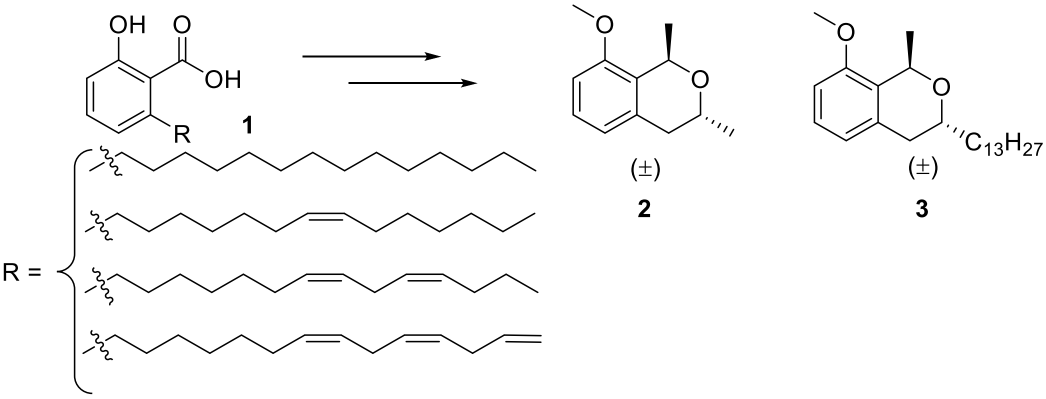

Figure 1 Synthesis of racemic isochromans **2** and **3** from bio-based anacardic acid **3**.

A number of the compounds synthesized were tested for antifungal and antibacterial activity. It was noted that a number of these showed interesting biological activity against Gram positive organisms, especially *B. cereus.*

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To investigate the antibacterial activities of Herbal extracts in laboratory condition and prepare a "Bio-disinfectant" using different combination of herbal extracts based on its antibacterial activity results

Thani Saud A M Al Thani, Mohammed Khalid Al Mutawaa, Dr J C Sharma [!]

Qatar Leadership Academy, Qatar
[!]**jsharma@qf.org.qa**

Abstract

As part of interdisciplinary research project, we worked on a project to develop "Bio-disinfectant" for our greenhouse plants using typical herbs. Firstly, we prepared a variety of herb extraction using various techniques, i.e., Fractional Distillation, Solvent Extraction separating funnel techniques, etc. The herbal extract was later used to conduct the anti-bacterial studies in the lab. we visited the Central Lab Unit (CLU) of the Department of Chemistry and Earth Science, Qatar University to understand the molecular structure of herbal extracts using advanced technologies. we worked with researchers to get the IR data for the herbal extracts using FTIR spectroscopy. IR data helped us to identify the active organic functional groups (mainly alcohols and carboxylic acids) in the herbal extracts. The anti-bacterial activities were studies under laboratories condition. Herbs were gathered from the school's herbal garden and used to take out extraction of 8 different crops (sage, lemon, ginger, clove, onion, thyme, garlic, mint, and vinegar) the extracts later, the extractions were diluted into 6 different concentrations (0%,20%,40%,60%,80%, and 100%). We took the bacteria from different surfaces such as tables, door handles, and the bacteria was turned into a solution then placed into petri dishes and spread using L-shaped rod. Small papers of different colors were dunked in different extractions and placed in the petri dishes to see the efficiency of it against the bacteria. The bacteria were cultured for 48 hours before the results were analyzed by measuring the diameter of the inhibition zone. Data analysis was collected based on the measurements. The inhibition zone of petri dishes was tested for different extractions and at different concentrations.

TOWARDS THE DESIGN OF ADVANCED MOF-BASED AIR DEHUMIDIFICATION MEMBRANES: MOLECULAR DYNAMICS STUDY OF WATER, NITROGEN, AND OXYGEN IN UIO-66 MOF

Laya Roustazadeh[1], **Panagiotis Krokidas**[2], **Othonas Moultos**[3], **Ioannis Economou**[1]

[1]*Chemical Engineering Department, Texas A&M University at Qatar, Doha, Qatar*
[2]*National Center for Scientific Research "Demokritos", Institute of Nanoscience and Nanotechnology, Molecular Thermodynamics and Modelling of Materials Laboratory, 15310 Aghia Paraskevi Attikis, Greece*
[3]*Engineering Thermodynamics, Process & Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Delft, The Netherlands*

E-mail: laya.roustazadeh@qatar.tamu.edu

A significant source of energy consumption in hot and humid regions is the dehumidification of conditioned air delivered to the building areas [1]. The conventional air dehumidification methods currently in practice are condensing moisture air dehumidification and desiccant absorption-based air dehumidification. Both methods are highly energy and cost-intensive. Therefore, new methods such as membrane air dehumidification have been attracting much interest thanks to their lower energy consumption and higher efficiency [2].

Metal-Organic Frameworks (MOFs) feature high porosity, uniform but controllable pore diameters, and the ability of surface functionalization. Due to these distinct characteristics, MOFs are gaining a lot of interest for separation processes [2]. MOFs separate the molecules by their size and shape or their interaction with the membrane material. UiO-66 is a recently-developed MOF that exhibits high thermal, mechanical, acidic, and water stability, and remains unaltered in water adsorption/desorption cycles [3]. There are several studies on the applications of UiO-66, such as carbon dioxide capture [4], storage and separation of short-chain hydrocarbons [5], and removal of warfare agents [6], which are mostly adsorption based. To design/optimize these processes, accurate knowledge of the diffusivities of the adsorbates is necessary. However, the studies on diffusion of confined molecules within UiO-66 pores are scarce, and present significant deviations from each other.

In this work, the diffusivity of the main species of humid air within the pores of UiO-66 is studied using MD simulations. These calculations were done on pure species first and then the diffusion of binary combinations of water/nitrogen and water/oxygen were studied. The final goal was the study of the ternary system of water, nitrogen, and oxygen at air composition and assess whether this MOF is a good material to be used as a dehumidification membrane for the air conditioning technology. The current results for pure species diffusion compare well with the existing experimental data, and the permeability and selectivity values found for the binary systems are in favor of the application. Also, the H-bond analysis done on the binary systems show no H-bonds formed between water and the MOF, however, there is a strong electrostatic interaction between the water molecules and the Zr nodes which hinders the water diffusion at lower loadings of water.

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TRANSITION METAL SCHIFF BASE AS POTENTIAL ANTIMALARIAL AGENTS AGAINST *PLASMODIUM SP.* INFECTION

Nur A. Z. Norazmi,[1,2,3] Nurul H. Abd Karim,[1] Prof. Masahiro Ebihara,[3] Nurul I. Hassan[1]
[1] Department of Chemical Sciences, Faculty of Science of Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Malaysia
[2]ACS UKM International Student Chapter, Universiti Kebangsaan Malaysia, 43600 Bangi, Malaysia
[3]Department of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University, 1-1 Yanagido, Gifu City 501-1193, Japan
E-mail: P107328@siswa.ukm.edu.my

Transition metal complexes have been studied extensively as a potential alternative treatment for numerous diseases, including malaria. Their ability to coordinate with ligands in a three-dimensional configuration allows the functionalization of groups altered according to targeted sites [1]. Schiff base compounds have demonstrated outstanding performance against several diseases and are often enhanced in the metal complex form [2]. This project introduces a series of tetradentate Schiff base metal complexes as potential antimalarial agents.

Six metal(II)-salphen complexes (nickel, copper and zinc) were prepared via condensation reaction of 2,5-dihydroxybenzaldehyde and o-phenylenediamine or 4-fluoro-o-phenylenediamine with respective metal(II) acetate. Fourier Transform Infrared (FT-IR), Nuclear Magnetic Resonance (NMR), and UV-Visible Spectroscopy were used to characterise the complexes. All synthesized complexes were evaluated for *in vitro* antiplasmodial activity using *P. falciparum K1* (Chloroquine-resistant) culture and cytotoxicity assay. *In silico* studies were conducted to predict the absorption, distribution, metabolism, excretion (ADME) and blood-brain barrier penetration and gastrointestinal absorption (BOILED-Egg method) profile of each complex with the aim of the determination of bioavailability.

The ADME and BOILED-Egg data suggested that the studied metal compounds can be used as potential therapeutic orally active drug. One of the complexes, Nickel(II) salphen with fluoro group was shown to have high antimalarial activity against chloroquine resistant *Plasmodium falciparum* K1 strain. The complex will be further tested against all types of human malaria parasites to determine its' efficiency and versatility.

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TRANSITION-METAL-FREE HOMOPOLYMERIZATION OF PYRROLO[2,3-D:5,4-D′]BISTHIAZOLES USING TURBO-GRIGNARD REAGENT

Attar Salahuddin[1], Dey Somnath[1], Manley Eric F[2], Moncho Salvador[1], Brothers Edward N[1], Bazzi Hassan S[1], Bronstein Hugo[3], Marks Tobin J[2], Heeney Martin[4], Schroeder Bob C[5] and Mohammed Al-Hashimi,*

[1]Department of Chemistry, Texas A&M University at Qatar, P.O. Box 23874, Doha, Qatar
[2]Department of Chemistry, Materials Research Center, and Argonne-Northwestern Solar Energy Research Center, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, United States.
[3]Department of Chemistry, University of Cambridge, Cambridge CB2 1EW, U.K.
[4]Department of Chemistry and Centre for Plastic Electronics, Imperial College London, Exhibition Rd, London, SW7 2AZ, U.K.
[5]Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, U.K.
E-mail: mohammed.al-hashimi@qatar.tamu.edu

Novel methods to synthesize electron-deficient π-conjugated polymers utilizing transition-metal-free coupling reactions for the use of nonfunctionalized monomers are attractive due to their improved atom economy and environmental prospective. Herein we describe the use of turbo-Grignard ^{i}PrMgCl·LiCl complex to afford thiazole-based conjugated polymers in the absence of any transition metal catalyst, that enables access to welldefined polymers with good molecular weights. The mechanistically distinct polymerizations proceeded via nucleophilic aromatic substitution (SNAr) reaction supported by density functional theory (DFT) calculations. This work demonstrates the first example of fully conjugated thiazole-based aromatic homopolymers without the need of any transition metal catalyst.

TREATED WASTEWATER REUSE FOR IRRIGATION IN BEKAA, LEBANON: QUALITY ASSESSMENT AND PUBLIC PERCEPTION

Tia Hajjar [1]
Supervised by Dr. Sandra Yanni [2]**, Rabi Mohtar**[2+3]**, Mey Jurdi**[4]**, May Massoud**[4]**, and Yaser Abunnasr** [1]

1 Department of Landscape Design and Ecosystem Management, Faculty of Agricultural and Food Sciences, American University of Beirut, Beirut, Lebanon.
2 Department of Agriculture, Faculty of Agricultural and Food Sciences, American University of Beirut, Beirut, Lebanon.
3 Biological and Agricultural Engineering and Zachry Department of Civil Engineering, Texas A&M University, Texas, USA.
4 Department of Environmental Health, Faculty of Health Sciences, American University of Beirut, Beirut, Lebanon.
E-mail: trh03@mail.aub.edu

In Lebanon, agriculture consumes 61% of the freshwater resources [2]. In this sector, an estimated water supply-demand gap of 25% is predicted to further increase with the elevated and unmet water demand and the exacerbating pressure on the water supply [4]. Consequently, integrated water resource management can sustainably help manage our water resources for agriculture and other sectors [3]. In particular, treated wastewater reuse (TWWR) is among the alternative water sources for irrigation to increase water availability and reduce the pressure on our freshwater resources. Despite the negligible water reuse situation in Lebanon and its numerous challenges, this non-conventional water source can be a sustainable option for water management because of its environmental, public health, and economic benefits [3,5]. Nonetheless, failing to ensure a safe-effluent quality leads to environmental and public health risks [7]. The Bekaa region is the primary agricultural area producing most of the country's irrigated crops [2]. The Bekaa also has several functional wastewater treatment plants (WWTPs) [6]. However, insufficient studies are available about their efficacy of treatment and their water reuse potential in irrigation in terms of the safety of the effluent's quality. Furthermore, successful reuse projects significantly depend on farmers and public acceptance of TWWR [1]. Unfortunately, the level of acceptance is overlooked in Lebanon [7,8].

Therefore, this study aims to determine the physical, chemical, and microbiological quality of TWW from Ablah and Zahle WWTPs in the Bekaa for reuse in irrigation and evaluate their environmental and public health risks. It will further investigate the willingness of (i) farmers in Zahle and Ablah and (ii) consumers from the Lebanese communities towards safe TWWR. It will also compare the actual risks of irrigating with the TWW of the studied WWTPs with the perceived risks of farmers and consumers regarding safe TWWR. The quality of water effluent grab samples was analyzed and will be compared with international guidelines for water reuse and irrigation. Two surveys were conducted targeting (i) the Lebanese population, aged 18 years and above, through social media platforms and (ii) randomly selected accessible farmers who can benefit from Zahle and Ablah WWTPs through face-to-face and telephone interviews. Data collected will then undergo statistical analysis (descriptive and analytical – multivariate logistic regression model).

This research is funded by the EU PRIMA under MAGO project.

TUNABILITY OF SIMPLE ELECTROLYTE INTERACTION, MECHANICAL AND SWELLING PROPERTIES IN HYDROGELS FABRICATED FROM TRIMETYLAMINEOXIDE (TMAO)–LIKE METHACRYLIC MONOMER.

Ruqaia Shoheeduzzaman,[1,2] Mirza Taha Baig[1,2] Peter Kasak,[1]

[1]*Center for Advanced Materials, Qatar University, Doha, Qatar.*
[2]*College of Arts and Science, Qatar University, Doha, Qatar*
Email: rh1805547@student.qu.edu.qa , mb1706996@student.qu.edu.qa peter.kasak@qu.edu.qa ,

Zwitterion polymeric materials are a benchmark for having a wide range of applications in the field of medicine such as biocompatibility of implants, drug delivery systems, biosensors and most importantly, preventing biofouling. Such applicable properties are conferred from balanced charge, highly ionic and large water swelling characteristics of such materials [1]. However, interactions with simple electrolytes often limit applications due to large swelling differences. In this study, zwitterion-based hydrogels with trimethylamine N-oxide-like (TMAO) motif were investigated. The TMAO motif is of interest to us since biomimetic TMAO is one of the most effective protein stabilizers and osmolyte [2]. Novel methacrylic TMAO-like monomer was synthesized and used for free-radical polymerization [3] with N,N’-methylenebis-acrylamide (BIS) as a crosslinker, ammonium peroxidedisulphate (APS) as photo-initiator, and N,N,N’,N’-tetramethylethylenediamine (TMDEA) as an accelerator for the hydrogel sample fabrication. Modulability of crosslinking density, applied monomer and monomer concentration allows for the tailoring of mechanical and swelling properties of resulted hydrogel samples. In addition to the modulation study of TMAO hydrogels, interaction with simple electrolytes was also investigated and will be presented. .

Acknowledgement

This contribution was made possible by the grant IRCC-2020-004 and QUST-1-CAM-2021-1.

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UTILIZING MODELING TOOLS TO DESIGN A REACTOR AND A CATALYST FOR DRY REFORMING OF METHANE

Murtaza Ali Khan,[1,2] Mohamed S. Challiwala,[1,2,3] Minhaj M. Ghouri, Anuj Prakash,[1] Anjaneyulu Chatla,[1] and Nimir O. Elbashir[1,2]

[1]*Chemical Engineering Program and Petroleum Engineering Program, Texas A&M University at Qatar, Doha 23874, Qatar*
[2]*TEES Gas & Fuels Research Center, Texas A&M University, College Station, Texas 77843, USA*
[3]*Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas 77843, USA*
Email: murtaza.khan@qatar.tamu.edu

Dry reforming of methane (DRM) is a catalytic reaction in which two greenhouse gases (CO_2 and CH_4) are converted to synthesis gas (a mixture of CO and H_2), an important precursor to produce various chemical products. DRM is highly attractive due to its ability to convert greenhouse gases; however more research is required to address its process challenges: (a) high energy requirement, (b) low synthesis gas quality, and (c) catalyst deactivation due to carbon formation. Nickel (Ni) catalyst is widely used for methane reforming and thus suitable for DRM as well. However, it is prone to carbon formation due to reactions like methane decomposition and Boudouard reaction causing deactivation. A novel bimetallic nickel-copper (Ni-Cu) catalyst was previously developed in our research group at an atomistic scale using density functional theory (DFT) approach to address the Ni catalyst's carbon formation challenge. The Ni-Cu catalyst provides significant carbon resistance and superior stability compared to the conventional Ni catalyst. The catalyst's performance was proven and validated experimentally in our laboratory's state-of-the-art bench-top reactor.

The scope of this work is to explore the scalability of the novel Ni-Cu catalyst using a mathematical modeling approach. The approach comprises of utilizing an existing one-dimensional (1-D) pseudo-homogeneous reactor bed model supported by lumped kinetics of a network of complex reactions that take place during DRM. This model was updated by including accountability of carbon formation and advancing further to account for detailed transport properties. The kinetics of Ni to Ni-Cu catalyst were scaled using a novel approach utilizing DFT and results in providing predictions for the bulk-scale kinetics performance in terms of carbon formation rates.

The experimental validation of the model was first tested using a conventional monoatomic Ni catalyst then later extended to predict the performance of the Ni-Cu catalyst. The 1-D model yielded results that match within an error margin of 5% with experimental data especially on CH_4 conversions. The developed 1-D model serves as a tool to predict the performance of the Ni-Cu catalyst at various reactor scales and to conduct future optimization and process intensification studies for DRM process by maximizing feed conversions.

Chemical Engineering Sciences and Fundamentals

^{13}C NMR Investigations and Order Parameters of Rod-Like Molecules with Terminal Phenyl and Thiophene Rings in Mesogenic Core§

A. A. Boopathi[a,b], Nitin P. Lobo[b,c], and
T. Narasimhaswamy[a,b,]

[a]Polymer Science and Technology,
[b]Centre for Analysis, Testing, Evaluation & Reporting Services (CATERS),
CSIR-Central Leather Research Institute, Adyar, Chennai-600020, India
[c]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.

Abstract

Rod-like mesogens with the rigid core constituted by a combination of phenyl and thiophene moieties reveal interesting orientational ordering behavior. In this article, four rod-like mesogens constructed with a terminal alkoxy chain on only one side of the mesogenic core with the other end terminated with either a phenyl or thiophene ring have been investigated using ^{13}C NMR spectroscopy. The mesogen with the terphenyl moiety in the core exhibited polymesomorphism with nematic, smectic C, and smectic I mesophases with very high clearing temperatures. The replacement of terphenyl with terthiophene moiety resulted in suppression of polymesomorphism, with only nematic mesophase being observed. Mesogens with single terminal thiophene connected to two phenyl rings in the core also showed only the nematic mesophase for both the possibilities of linking the core to the thiophene ring at the 2- and 3- positions. One- and two- dimensional ^{13}C NMR spectra have been obtained in the mesophases from which the alignment induced chemical shifts of the ring carbons and ^{13}C-^{1}H dipolar couplings, as well as the local order parameters, have been obtained. The considerable difference in ^{13}C chemical shifts and the ^{13}C-^{1}H dipolar couplings of thiophene ring with change in position of the linking unit is attributed to the difference in the order parameters of the thiophene moiety between the two cases. The data obtained on the ordering of phenyl and thiophene rings in the core units offered information into the effect of replacing the phenyl ring with the thiophene ring. So also, the change of position of the link to the thiophene moiety provided important insights into the orientational behavior in the liquid crystalline phase and on the molecular structure.

Keywords (6 only): Rod-like mesogens, smectic I phase, ^{13}C-^{1}H dipolar couplings, SLF, Order Parameters, ^{13}C NMR

A KINETIC MODEL FOR ANODIC DISSOLUTION OF CARBON STEEL IN THIOSULFATE-AMMONIUM CHLORIDE SOLUTIONS

Prince Kumar Baranwal[1, 2]

[1]*Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar*

[2]*Department of Chemical Engineering, Indian Institute of Technology Guwahati, Guwahati, Assam, India*

E-mail: pbaranwal@hbku.edu.qa

Carbon steel (CS) is one of the most widely preferred and economic materials employed in oil and gas industry. However, CS experiences aggressive corrosion due to the presence of acids, chlorides or sulfur corrosive species that leads to predominant problems in industries [1-2]. In the present work, a systematic mechanistic investigation was attempted to understand the effect of sodium thiosulfate ($Na_2S_2O_3$) on CS dissolution behavior in ammonium chloride (NH_4Cl) solution by means of anodic polarization and electrochemical impedance spectroscopy (EIS) methods. The surface morphology was analyzed using scanning electron microscopy and the chemical composition of the corrosion products formed on the surface were identified with energy dispersive spectroscopy and X-ray photoelectron spectroscopy. The polarization and EIS curves indicated a considerable increase in the dissolution rate of CS with addition of thiosulfate to the ammonium chloride solution. The EIS measurements conducted at three *dc* overpotentials with respect to (w.r.t.) open circuit potential (OCP), as shown in Figure 1, depicted formation of two-time constants in each case. The results indicate that the total impedance decreases with increase in overpotential, implying no formation of strong passive layer on the CS surface. Based on the experimental findings, electrical circuit combined with reaction mechanism analysis approach were utilized to determine the kinetic reaction mechanism of CS dissolution. A multi-step reaction mechanism with two dissolution paths and adsorbed species (Fe^{2+}) was proposed. The kinetic parameters were retrieved for the proposed mechanism using sequential quadratic programming. The surface coverage and dissolution rate were also computed from these kinetic parameters.

Keywords: Carbon steel corrosion, ammonium chloride, thiosulfate, impedance, kinetic reaction mechanism

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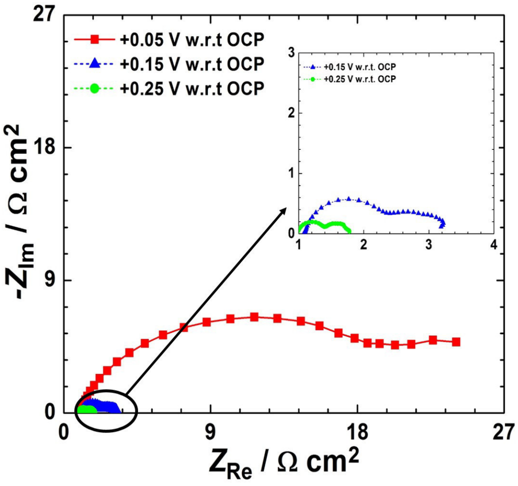

Figure 1: Nyquist plot for CS dissolution in 20 wt.% NH_4Cl containing 0.1 M $Na_2S_2O_3$ solution at three different overpotentials w.r.t. OCP

AN EMPIRICAL CORRELATION-BASED MODEL TO PREDICT SOLID-FLUID PHASE EQUILIBRIA FOR FLUE GAS MIXTURES

Hani Ababneh [a] and **Shaheen A. Al-Muhtaseb [b]***

Department of Chemical Engineering, College of Engineering,

Qatar University, 2713 Doha, Qatar

[a] *ha1805750@student.qu.edu.qa*,

[b] *s.almuhtaseb@qu.edu.qa*

**Corresponding author*

Abstract

Flue gases resulting from the combustion of fossil fuels are among the major sources of carbon dioxide (CO_2) and other greenhouse gases emitted to the atmosphere. Flue gases are a mixtures of water vapor (H_2O), nitrogen (N_2), particulates, heavy metals and acid gases (such as CO_2 and H_2S). Additionally, in case of incomplete combustion, flue gases contain carbon monoxide (CO) and volatile organic compounds (VOCs) [1]. The typical composition of flue gases emitted from natural gas-fired power plants is 8-10% CO_2, 18-20% H_2O, 2-3% O_2, and 67-72% N_2 [2].

The most widely used technology in the industry to capture CO_2 is the solvent (e.g., amine)-based absorption technology. However, this technology suffers from high energy requirements and high cost for maintenance and operation [3]. The cryogenic separation technologies have caught the attention of engineers and scientists as a new alternative technology to capture CO_2 from flue gas mixtures. The cryogenic separation offers few advantages over the traditional CO_2 capturing technologies; including a lower environmental footprint and eliminating the need for solvents, which can make it less expensive to build and operate when compared with amine scrubbing [4]. Cryogenic separation is a physical process that relies on the differences in volatilities between CO_2 and the other gases in flue gas to separate CO_2 at very low temperatures [5]. Some cryogenic separation technologies (such as the Controlled Freezing Zone, CFZ^{TM}) depend on the solid phase formation to improve the separation process. Therefore, to design cryogenic separation process units and equipment involving such solid phase, thermodynamic equilibrium data of vapor-liquid equilibrium (VLE), solid-liquid equilibrium (SLE), solid-vapor equilibrium (SVE), and solid-liquid-vapor equilibrium (SLVE) are required.

The main aim of this study is to develop an empirical predictive model based on Peng-Robinson equation of state (PR EoS), with fugacity expressions, that is able to predict the SLVE for the ternary system of N_2-O_2-CO_2 (to represent a sample flue gas mixture) at wide range of pressures and temperatures. The importance of this study is that it is provides researchers and the industry with an important tool to predict of the ternary SLVE behavior of flue gases, without the need for experimental measurements, which in turn optimizes the budget and time of such communities.

COREFLOOD CHROMATOGRAPHY IN LIMESTONES

Samuel Fontalvo[1], **Maxim Yutkin**[1], **Ksenia Kaprielova**[1], **Tadeusz Patzek**[1]

[1]Ali Al-Naimi Petroleum Engineering Research Center, King Abdullah University of Science and Technology, Saudi Arabia

E-mail: samuel.fontalvoguzman@kaust.edu.sa

Abstract

Improving recovery from carbonate oil reservoirs is paramount to uninterrupted energy supply and any future energy transition. One of the aspects of recovery improvement deals with crude oil-brine-carbonate rock interface chemistry. Despite decades of research, the understanding of this area are limited. In this work, we study surface chemistry of calcium carbonate rocks *via* series of coreflood experiments and modeling.

Coreflood experiments are performed on 1.5” by 3” Indiana limestone core plugs. Chloride-ion tracer-test experiments allows characterizing hydrodynamic dispersion. Effluent is collected each 0.1 pore volume (PV), for at least 3 PV. Concentration history data are fitted with the analytic solution.

Next, we study adsorption of different surfactants: negatively charged sodium dodecyl sulfate (SDS), positively charged benzalkonium chloride, and neutral hexadecanol. Surfactant adsorption is then modeled using open-source software, PHREEQC. In our 1D transport model, we account for calcium carbonate dissolution, bulk aqueous speciation, dispersion, surfactant adsorption, and ion exchange on calcium carbonate surface.

Indiana limestone core plugs are highly heterogeneous and have high hydrodynamic dispersion, which leads to difficulties in interpreting adsorption. Therefore, we posit that tracer experiments are vital for meaningful interpretation of adsorption and ion exchange results. At the same time, even though Indiana limestone exhibits surprisingly low specific surface area and adsorption capabilities, it is enough to affect bulk calcium and sodium concentrations through ion exchange.

Calcium carbonate surface accumulates both negative and positive ions in the β-plane depending on brine composition. Therefore, we expect that surfactant adsorption would depend on brine composition. We investigated adsorption of SDS in different brines. In NaCl-based brines, we find that SDS adsorbs weakly. In Na2CO3 brine, SDS adsorption is undetectable, as expected. Conversely, we expect higher adsorption of SDS in CaCl2/MgCl2-based brines. Models that include dispersion, calcite dissolution, bulk speciation, Na/Ca ion exchange can explain the experimental adsorption data.

EMERGING TRENDS IN BIODIESEL PRODUCTION TECHNOLOGY

N.Kapilan,[1] **Nithin K C,**[1] **Chiranth K N**[1]

1Department of Mechanical Engineering, Nitte Meenakshi Institute of Technology,
Bangalore 560064, India
E-mail: kapilan.n@nmit.ac.in

The renewable energy sources are getting attention in recent years due to fossil fuel depletion and climate change and global warming issues related to burning of fossil fuel. The biodiesel is considered as a potential replacement to fossil diesel [1]. The first- and second-generation biodiesel are produced from edible and non-edible feedstocks respectively. The microwave-assisted oil extraction results in better oil quality and reduces production time and cost. The third-generation biodiesel is produced from animal fat, waste cooking oil and algae. The fourth-generation biodiesel work is related to genetic engineering to enhance the oil yield using genetically modified feedstock [2]. The heterogeneous catalyst has few better charactertics compared to homogenous catalyst. It is suggested that the heterogeneous catalyst can be produced from sustainable alternative material [3]. For example, a heterogeneous solid acid catalyst can be produced from fast pyrolysis of rice straw. The reusable catalysts are developed in recent years to reduce operating cost [4]. Significant research work has been carried out to develop catalyst which is low cost and also sustainable. A multi-step transesterification is developed to produce biodiesel from low cost feedstock [5].

The major disadvantages of homogeneous alkali catalysts are overcome by the development of Ionic liquids. This catalyst has unique properties such as better solubility, non-volatile, better operating temperature range and structure tunability [6]. In recent years, the membrane technology is used for the separation and purification of biodiesel. It is reported that the micro- and ultrafiltration membranes result in better separation of biodiesel and glycerol [7]. The water washing has several disadvantages and hence dry washing method is developed. It’s environmental impact and contamination is lesser than the water wash. The commercial adsorbent produced from industrial process may not be sustainable and hence sustainable methods and materials are used to produce adsorbent. The material such as rice husk, coconut fiber, water hyacinth fiber and sawdust can be used to produce bioadsorbents for the purification of biodiesel. It is reported that the sawdust is the best alternative bioadsorbent for dry purification of biodiesel and also it has lower environmental impact [8]. From this work, we conclude that there are several opportunities to develop new methods and catalytic materials for the biodiesel production, biodiesel separation, purification and drying.

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INFLUENCE OF STRUCTURE AND HETEROMETAL ON PROPERTIES OF A FAMILY OF POLYOXOMETALATES (POMS) – A HYDROLYTIC STUDY

Thompson Izuagie,[1,2] Daniel Lebbie[2] and R. John Errington[2]

[1]Department of Chemistry, Sokoto State University, Sokoto, Nigeria
[2]Newcastle University Polyoxometalate Laboratory (NUPOM),
Newcastle upon Tyne, UK
*Email:*Tomyi2012@yahoo.com

This paper uses a blend of experimental observations and DFT calculations to understand the influence of type of heterometal and POM structure (Lindqvist and Keggin) on the solution properties of a family polyoxometalates. Previous studies on the Lindqvist POMs revealed some interesting variations in the hydrolytic and protonation behaviours of the TiW_5 and SnW_5 systems[1]. This paper extends the study to the Keggin series, $TiPW_{11}$ and $SnPW_{11}$. The POMs were synthesized *via* non-aqueous methods developed in Newcastle and characterized using CHN elemental microanalysis, FT-IR and multinuclear NMR (^{1}H, ^{17}O, ^{31}P, ^{119}Sn and ^{183}W) spectroscopies. The insights gained enabled the characterization of $[(MeO)SnPW_{11}O_{39}]^{4-}$ and $[(\mu\text{-}O)(SnPW_{11}O_{39})_2]^{8-}$ – two new members of the Keggin family. Comparison of the Lindqvist, $[(MeO)MW_5O_{18}]^{3-}$ and Keggin, $[(MeO)MPW_{11}O_{39}]^{4-}$ (M = Sn, Ti) hydrolysis reactions showed that the highest energy barrier was for $[(MeO)TiPW_{11}O_{39}]^{4-}$ while the lowest was for $[(MeO)SnPW_{11}O_{39}]^{4-}$. Additionally, the tin-substituted anions in each family were observed to be the most stable. The study provided new data for extending available ^{17}O NMR models on the POM families and contributes towards establishing a versatile platform for development in POM science.

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LOW-TEMPERATURE REVERSE WATER-GAS SHIFT REACTION OVER TRANSITION METAL-LOADED LANTHANUM OXIDE NANOPARTICLE CATALYSTS

Parisa Ebrahimi, Anand Kumar* and Majeda Khraisheh

Department of Chemical Engineering, Qatar University, Doha, P O Box 2713, Qatar

E-mail: pebrahimi@qu.edu.qa

Reverse Water Gas Shift (RWGS) reaction is considered as one of the most appealing processes for converting CO_2 to CO, where after mixing with H_2 as syngas, it can be put into a well-established Fischer-Tropsch process to produce fuels and chemicals of choice [1]. At low temperatures, however, it competes with the highly exothermic CO_2 methanation process, which produces methane and lowering CO yield [2]. Therefore, developing selective catalysts for the RWGS reaction that can result in cost-effective CO_2 hydrogenation remains a challenging task [3].

Several studies have been carried out to create catalysts based on transition metals such as Cu and Ni that are also effective catalysts in the WGS process, and the active catalysts in the WGS reaction are also efficient in the RWGS reaction [4]. Although Ni has a strong hydrogenation catalytic activity that is more selective for methane production than CO, oxide-supported Ni nanoparticles with high oxygen capacities are being studied for the RWGS [5]. CO_2 titration reveals that an oxide like La_2O_3 has a large number of basic sites and is thermally stable, making it an excellent CO_2 absorption support [6]. The role of reducible lanthanum support deposited with Cu and Ni active metals using solution combustion method (SCS) and its function in a tubular packed bed reactor for the RWGS reaction is investigated in this work. Figure 1 indicates that increasing the temperature enhances CO_2 conversion, with a maximum CO_2 conversion of 57% and 68% at 600°C for CuLa and NiLa, respectively, which were stable for 24 hours.

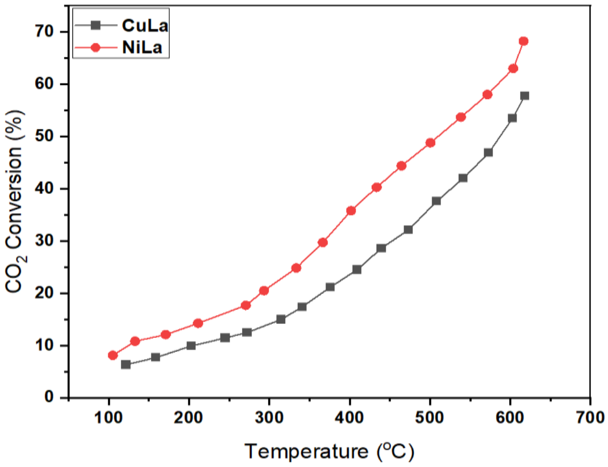

Figure 1. CO_2 conversion to CO during the RWGS reaction over CuLa and NiLa

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METHANE DECOMPOSTION OVER COMBUSTION SYNTHESIZED Fe/SiO_2 CATALYSTS

Assem Taha,[1] Muftah El-Naas,[1] Dharmesh Kumar,[2] Anand Kumar[3]

[1]*Gas Processing Center, Qatar University, Doha, P O Box 2713, Qatar*
[2]*Qatar Shell Research and Technology Center (QSRTC), Doha, P O Box 3747, Qatar*
[3]*Department of Chemical Engineering, Qatar University, Doha, P O Box 2713, Qatar*
Email: akumar@qu.edu.qa

Methane decomposition is one of the most promising methods to convert methane to carbon, hydrogen and hydrocarbons [1]. As the most reduced carbon molecule, methane is an excellent carbon and energy source. However, it is the most stable and unreactive alkane without functional groups prone to chemical attacks, and hence a high energy is required for methane activation and conversion [1-3]. Herein, we explore the utilization of Fe/SiO_2 catalysts to decompose methane to hydrocarbons by optimizing the catalysts and reaction conditions. For this purpose, Fe/SiO_2 catalysts were synthesized by solution combustion synthesis method (SCS) by varying Fe loading and amount of fuel during the synthesis process. The prepared catalysts were tested in a quartz tube fixed bed reactor at temperatures ranging from 750°C to 1100°C and atmospheric pressure. The effluent gases were passed through an online GC for detecting the gaseous hydrocarbon products. A dry ice trap was installed to collect the liquid products to be analyzed offline by GCMS.

Catalytic results indicate that iron loading, fuel amount during synthesis, and calcination temperatures (600°C, 1100°C and 1530°C) have considerable impact on the conversion of methane and hydrocarbon selectivity. A high calcination temperature tends to be more selective for aromatics, whereas a low calcination temperature favors carbon formation. A consistent conversion-selectivity correlation was observed indicating higher conversion conditions being favorable for carbon formation, whereas catalysts and reaction parameters can be tuned to obtain varying hydrocarbon/carbon selectivity at low methane conversion conditions. In addition, catalysts were modified by acid leaching and doping with Cs (ion-exchange) to increase hydrocarbon selectivity. Characterization techniques like SEM, Raman, XRD, TGA, BET surface Area, XPS, TPO, TPR and CHN analysis were used to gain insight into the physio-chemical properties of the catalysts that are correlated with catalytic performance.

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Ni-MgO BASED NOVEL CATALYSTS PREPARED BY COMBUSTION SYNTHESIS FOR CO_2 AND METHANE REFORMING

E.E. WOLF[1]

With: V. Danghyan[1]*, A. Mukasyan*[1] *and A. Kumar*[2]

[1]*Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, USA.*

[2]*Department of Chemical Engineering, Qatar University, Doha, Qatar.*

In this talk we present mechanistic aspects of the solution combustion synthesis of high surface area Ni-MgO solid solutions as highly effective and stable catalysts for the dry reforming of methane (DRM) with CO_2, two major greenhouse gases.

A novel route for catalyst preparation, based on the solution combustion synthesis (SCS) method, has been investigated. In SCS, an aqueous solution containing a metal nitrate precursor (oxidant) is mixed with glycine (fuel) and dried to obtain a thick reactive gel, which is preheated until at a certain temperature the highly exothermic combustion reaction is initiated resulting in the formation of metal oxides. A modification of SCS was used by impregnating the reactive solutions into a cellulose paper, referred as paper assisted combustion synthesis (PACS).

During the synthesis, the combustion reaction exothermicity, temperature, and front propagation velocity were monitored by high-speed Infrared thermography and differential scanning calorimetry (DSC). The Ni-MgO formed solid solutions were characterized with textural (BET, SEM), structural (XRD, TPR, TEM), and surface analysis (XPS) techniques. Activity and stability of catalysts during the DRM were studied as a function of reaction temperature, time on stream (TOS), carbon deposition, and the reaction turnover frequency (TOF) was evaluated at differential methane and CO_2 conversions.

NiOMgO catalysts with 10, 20 and 30% Ni concentration were first prepared by SCS. All synthesized powders formed NiOMgO solid solutions with surface areas of up to 37 m^2/g, which were inactive for DRM. They became active upon reduction at 600 ^oC, due to the segregation Ni atoms to the surface of the solid solutions, forming crystallites containing the active sites. On 20%Ni-MgO reduced catalyst, methane conversion reached about 50% at 600 ^oC, however, there was also carbon accumulation of about 80 wt.% after about 2 hours of TOS.

Unlike to SCS, PACS synthesized Ni-MgO solid solutions exhibited much higher surface areas, partly because during combustion Mg^{2+} ions strongly catalyzed cellulose pyrolysis, creating a porous media, which acted as a template to the NiO-MgO solid solutions. The 10%NiOMgO-PACS catalyst exhibited the highest surface area of 153 m^2/g compared to only 23 m^2/g prepared by SCS method. At 600 ^oC, the 10%NiOMgO-$PACS_R$ catalyst exhibited methane conversion close to equilibrium and significantly inhibited carbon deposition (~3 wt.% during 24 h TOS), thus increasing the catalyst's stability. The higher activity and stability of the 10%Ni-MgO catalyst is attributed to the higher dispersion and smaller size of Ni crystallites formed during the PACS synthesis, and the formation of a higher amount of Ni^{3+} surface site defects (2).

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