



ND Energy

**RESEARCH
SYMPOSIUM
POSTER SESSION**

April 18, 2018

1:00pm to 3:00pm

**Lower Level Dining Room,
McKenna Hall**

***Celebrating contributions to energy
research at Notre Dame***

ROSTER OF RESEARCHERS

#	Researcher	Project Title	Advisor	Dept.
1	Tyler Spano	Investigation of Uranium Dioxide Fuel Pellets for Nuclear Forensic Applications	Antonio Simonetti	CEEES
2	John Hoffman	Dual-Functionalized Nanofiltration Membranes for Water Purification	William Phillip	CBE
3	Trevor Demille	Light Mediated Growth of Noble Metal Nanostructures on ZnO Tetrapods	Svetlana Neretina	AME
4	Brooke Stemple	Enhanced ionic liquid tolerance of <i>Yarrowia lipolytica</i> through evolutionary engineering for simultaneous saccharification and fermentation of lignocellulosic biomass	Na Wei	CEEES
5	Tuphan Devkota	Nanostructure Acoustic Mode Damping in Liquid Environments	Gregory Hartland	Chemistry
6	Yaofa Li	Ensuring Long-Term Security of Stored CO ₂ : Fundamental Studies of the Multiphase Flow of Water and Liquid/Supercritical CO ₂ in 2D Heterogeneous Porous Micromodels	Kenneth T. Christensen	AME
7	Rebecca Carter	Rare earth element interactions with UO ₂	Amy Hixon	CEEES
8	Mark Summe	Structure-performance relationships and transport mechanisms of charge mosaic membranes	William Phillip	CBE
9	Randal Marks	Protection of MoS ₂ nanosheets from dissolution by aqueous oxidants using graphitized carbon	Kyle Doudrick	CEEES
10	Yolanda Bonita	Catalytic Applications of Bimetallic Ruthenium Molybdenum Phosphide for Selective Furfural Hydrogenation	Jason Hicks	CBE
11	Felipe Tagle	A Multi-Level Skew-t Stochastic Generator for Assessing High-Resolution Wind Energy Resources in Saudi Arabia	Stefano Castruccio	ACMS
12	Samuel N. Perry	Thermodynamics and structural complexity of sodium uranyl sulfate minerals with unusual structural topologies	Peter Burns	CEEES
13	Nick Kempf	A robust high-sensitivity scanning thermal probe for simultaneous microscale thermal and thermoelectric property mapping	Yanliang Zhang	AME
14	Andrew Schranck	An investigation of the effect of urine compounds on electrochemical oxidation of urea using a nanostructured nickel cobaltite catalyst	Kyle Doudrick	CEEES

#	Researcher	Project Title	Advisor	Dept.
15	Feng Gao	Charge Patterning Affects Ion Transport Through Charge-Mosaic Membranes	William Phillip	CBE
16	Corinne Dorais	Development of a new uraninite reference material for nuclear forensic analysis at high spatial resolution	Antonio Simonetti Amy Hixon	CEEES
17	Suzanne M. Neidhart	Morphology Dependence of Thermal Conductance in Gold Nanoparticle Systems	J.D. Gezelter	Chemistry
18	Yunsong Pang	Functionalized Graphene Enables Highly Efficient Solar Thermal Steam Generation	Tengfei Luo	AME
19	Sarah Hickam	Dissolution of uranium dioxide in uranyl peroxide cluster-forming conditions	Peter Burns	CEEES
20	Hansheng Ye	Investigation of the Effect of Growth Temperature on Deep Levels in GaAs for Photovoltaics	Patrick Fay	EE
21	Tanner Corrado	Synthesis and characterization of new polysulfones containing bulky bridging moieties for gas separation membranes	Ruilan Guo	CBE
22	Rebecca Scheidt	Modulation of Charge Recombination in CsPbBr ₃ Perovskite Films with Electrochemical Bias	Prashant Kamat	Chemistry
23	Hanyu Ma	DFT and Microkinetic Comparison of Pt, Pd and Rh(111) for Catalytic Ammonia Oxidation	William Schneider	CBE
24	Haylie Lobeck	Transformation of Uranyl Phosphate and Arsenate Minerals to Soluble Nanoscale Cage Clusters	Peter Burns	CEEES

Department Key

ACMS – Applied and Computational Mathematics and Statistics

AME – Aerospace and Mechanical Engineering

CBE – Chemical and Biomolecular Engineering

CEEES – Civil and Environmental Engineering and Earth Sciences

Chemistry – Chemistry and Biochemistry

EE – Electrical Engineering

Investigation of Uranium Dioxide Fuel Pellets for Nuclear Forensic Applications

Dr. Tyler Spano

Department of Civil and Environmental Engineering and Earth Sciences

College of Engineering

Advisor: Antonio Simonetti, Associate Professor and Director of Graduate Studies,
Department of Civil and Environmental Engineering and Earth Sciences

Abstract

A comparative investigation of the trace element compositions and structural properties for two uranium dioxide fuel pellets was conducted for nuclear forensic applications. One of the fuel pellets probed in this study consists of natural U (0.71 wt% ^{235}U) and the other contains enriched (3.98 wt% ^{235}U) UO_2 . Trace element abundances were determined utilizing solution mode inductively coupled plasma mass spectrometry (SM-ICP-MS). Cr, Mo, W, Co, and Ni impurities were observed in both fuel pellets, which likely originate from fabrication processes. Additionally, Zr was detected in the fuel pellet of natural U isotopic abundance. Structural properties of the UO_2 fuel pellets were examined using powder X-ray diffraction (pXRD) and Raman spectroscopy. Peak splitting, likely resulting from reduction of cubic symmetry in the UO_2 structure, was detected in the pXRD patterns for the fuel pellets. Peak broadening of the T_{2g} U-O stretching vibrational mode was observed in the Raman spectra of both fuel pellets and the magnitude of broadening may correspond to differential aging of the two materials. In addition, X-ray fluorescence spectroscopy was used to characterize the homogeneity of the fuel pellets, and non-traditional isotope signatures (e.g., B, Ca, Fe) were explored for the purpose of establishing novel nuclear forensic methodologies.

Dual-Functionalized Nanofiltration Membranes for Water Purification

John Hoffman, Ph.D. Candidate

Department of Chemical and Biomolecular Engineering

College of Engineering

Advisor: William Phillip, Associate Professor, Department of Chemical and Biomolecular Engineering

Abstract

As interest in decentralized water treatment units that enable localized water reuse grows, the development of nanofiltration (NF) membranes as a complementary technology to reverse osmosis membranes has gained traction. Furthermore, the use of advanced materials (e.g., graft copolymers), which form uniform nanoscale pores that are decorated with chemical moieties that provide a ready means for post-assembly functionalization, as membrane precursors are further expanding the potential range of membrane applications. For example, the incorporation of charged functionalities increases ion rejection by NF membranes due to repulsive electrostatic interactions. The main drawback and continued hurdle in the development and application of NF membranes is the process of fouling. Attractive dispersive, electrostatic, and hydrodynamic interactions between dissolved solutes and the membrane leads to the attachment and accumulation of material on the surface of the membrane, which reduces the throughput and performance. This study evaluates novel NF membranes that exhibit both high ion rejection and high fouling resistance. Poly(acrylonitrile-*r*-oligo(ethylene glycol) methyl ether methacrylate-*r*-glycidyl methacrylate) P(AN-*r*-OEGMA-*r*-GMA) is the parent polymer of this study, in which an epoxide ring open reaction of the GMA pore wall moiety leads to multiple functionalization avenues. A dual functionalized membrane containing both ion-selective and anti-fouling functionality is studied through the controlled deposition of propiolic acid onto the membrane using Electrohydrodynamic Jet (E-Jet) printing. This copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction occurs rapidly, leading to a penetration depth determined by the amount of deposited solution. This select layer achieves an anti-fouling character through an EDC coupling reaction of 1H,1H-Perfluorooctylamine. The layer not exposed to propiolic acid is then functionalized through a CuAAC reaction of propargyl amine. When challenged with a 0.5 g/L Bovine Serum Albumin (BSA) solution, these membranes express increased anti-fouling properties, experiencing a 10% decrease in permeability after 50 hours of exposure, compared to 40% decrease for a fully charged membrane during the same period. These membranes also see a 70% increase in rejection of MgCl₂ compared to a non-charged membrane.

Light Mediated Growth of Noble Metal Nanostructures on ZnO Tetrapods

Trevor Demille, Ph.D. Candidate

Department of Aerospace and Mechanical Engineering

College of Engineering

Advisor: Svetlana Neretina, Associate Professor, Department of Aerospace and Mechanical Engineering

Abstract

As a wide bandgap semiconductor exhibiting high electron mobility, room temperature luminescence, and piezoelectricity, ZnO has garnered intense interest. Its relevance has been further heightened by the ability to synthesize intricate geometries on both the nano- and micro-scales. The ZnO tetrapod, with its four arms connected to a central core, is a morphology of intense interest due to potential applications in electronics, sensing, biomedicine, catalysis, and composites. With a high Young's modulus, the ability to withstand high temperatures, and the capability to be produced in bulk quantities from earth abundant materials, ZnO tetrapods can act as an inexpensive structural support. The formation of metal nanostructures on micrometer size ZnO tetrapods is particularly intriguing from this standpoint in that there is the potential for a coupled response at the semiconductor-nanometal interface. Promoting metal nanostructure growth on the tetrapods can, however, prove challenging since the chemical environments used in many colloidal syntheses attack the ZnO surface. Light-mediated solution-based growth modes, however, present a possible alternative since they can be carried out at room temperature under relatively mild reaction conditions. Here, we describe the light-mediated synthesis of Au, Ag, Pt, Pd, Cu, Ir, Ru and Rh nanostructures on ZnO tetrapod supports. The supported structures are then assessed as catalysts and photocatalysts in the catalytic reduction of 4-nitrophenol by borohydride.

Enhanced ionic liquid tolerance of *Yarrowia lipolytica* through evolutionary engineering for simultaneous saccharification and fermentation of lignocellulosic biomass

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College of Engineering

Advisor: Na Wei, Assistant Professor, Department of Civil and Environmental Engineering and Earth Sciences

Abstract

Lignocellulosic biomass is the largest, renewable feedstock on the planet. However, the recalcitrance of lignocellulose materials is the main limitation of biomass processing, thus requiring intensive pretreatment processing to fractionate cell wall constituents. Ionic liquids (IL) are environmental benign with the ability to disrupt the bonds between cellulose, hemicellulose and lignin thus reducing cellulose crystallinity, allowing for easy recovery of cellulose and greater enzymatic hydrolysis compared to conventional dilute acid treatment. Unfortunately, applications to scale-up biorefinery are limited due to multiple expensive IL recovery and separation steps. This prompted investigation into a compatible enzymatic and microbial biocatalyst system to carryout simultaneous saccharification and fermentation (SSF) that can function in the ionic liquid environment as IL-pretreated biomass still contains 10-20% of IL carryover during SSF. Enhancing IL tolerance in an efficient microbial biocatalyst can reduce the need for extensive washing steps of the pretreatment products and reduce cost while increasing efficiency. Biological conversion of cellulosic biomass to fuels and valuable chemicals through enzymatic hydrolysis of cellulose offers the potential for higher yields, higher selectivity, lower energy costs and milder operating conditions than chemical processes. However, it is difficult to develop microbial biocatalysts that can survive and thrive in the IL environment, as well as perform efficient biotransformation under these intense, high salt conditions. In an effort to obtain a more vigorous microbial biocatalyst system we have used evolutionary engineering to develop a strain of *Yarrowia lipolytica* with a robust metabolism that can continue to grow at a competitive growth rate in an intense environment of 14% IL compared to the 10% IL the wildtype strain can survive in. *Yarrowia* is known for its ability to secrete copious amounts of proteins, organic acids and other valuable products and is an oleaginous yeast that can accumulate lipids at up to 80% of dry cell weight. Growth rate analysis of *Yarrowia* growing in liquid shake flask cultures possessing IL up to 14% showed an increased relative specific growth rate of the evolved strain, YIL16, with the potential to perform biotransformation in higher IL concentrations. Genomic analysis of the evolved strain as well as the wildtype was carried out using Whole Genome Sequencing (WGS) for further characterization of genotypes allowing for enhanced IL resistance. As well, lipids were extracted for analysis of fatty acid content and understanding the potential of biolipid production of the evolved strain. Cell physiology was also characterized using light microscopy for greater understanding of cell physical and morphological changes in response to IL stress. Overall, the evolution of *Yarrowia* to perform biotransformation in the intense IL environment promotes the opportunity for enhanced biofuels and bioproducts produced during SSF with the improved use of renewable lignocellulosic biomass as an abundant and renewable feedstock.

Nanostructure Acoustic Mode Damping in Liquid Environments

Tuphan Devkota, Ph.D. Candidate

Department of Chemistry and Biochemistry

College of Science

Advisor: Gregory Hartland, Professor, Department of Chemistry and Biochemistry

Abstract

Ultrafast laser excitation can generate acoustic vibrations in metal nanostructures. Acoustic vibrations transfer energy in the particle to the environment via the emission of sound waves. The effect of the environment on the acoustic vibrations in nanostructures has been investigated and the studies show that the local environment has a very little effect on the vibrational periods. In contrast, the lifetimes of acoustic vibrations are considerably affected by the local environment. We investigated the damping of acoustic vibrations in Au nanowires supported on a glass coverslip as well as suspended over the trenches in different liquid environments using transient absorption spectroscopy. We observed a significant decrease in the lifetimes of acoustic vibrations after immersing into a liquid whereas the frequencies of the vibrations remain unaffected. For the supported nanowires, the damping is mainly controlled by the acoustic impedance mismatch between the particle and its environment while the damping is more complicated in case of the suspended nanowires. The results are potentially useful to understand when the high frequency vibrations of nanostructures can be used to probe the viscoelastic properties of liquids and vice versa.

Ensuring Long-Term Security of Stored CO₂: Fundamental Studies of the Multiphase Flow of Water and Liquid/Supercritical CO₂ in 2D Heterogeneous Porous Micromodels

Dr. Yaofa Li

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College of Engineering

Advisor: Kenneth T. Christensen, Professor, Collegiate Chair in Fluid Mechanics and Department Chair, Department of Aerospace and Mechanical Engineering; Concurrent Professor, Department of Civil and Environmental Engineering and Earth Sciences

Abstract

Carbon capture and sequestration (CCS) is a viable technology for reducing carbon emissions from large CO₂ sources, such as fossil fuel thermal power plants. It represents an essential component in the battle against global climate change coupled with other “clean” energy approaches. In CCS, it is desired to capture CO₂ at the source and store it in geological formations, such as saline aquifers for geologically significant time periods. Central to this goal is accurately predicting both the fidelity of candidate storage sites pre-injection of CO₂ and its migration post-injection. Despite its importance in predicting CO₂ migration, our fundamental understanding of the coupled flow dynamics of CO₂ and water in complex geologic media still remains limited, especially at the pore scale. Recently, studies have been carried out in 2D homogeneous micromodels with the micro-PIV technique, highlighting the importance of inertial effects and local pressure gradients, especially during the burst events at pore scale, which plays a defining role in CO₂ transport. To this end, the pore-scale flow of water and liquid/supercritical CO₂ is investigated under reservoir-relevant conditions, over a range of wettability conditions in 2D heterogeneous micromodels that reflect the complexity of a real sandstone. Microscopic particle image velocimetry (micro-PIV) and high-speed fluorescent microscopy, complemented by a fast differential pressure transmitter, allow for simultaneous measurement of the flow field within and the instantaneous pressure drop across the micromodels. The work, for the first time, incorporates both real reservoir-relevant conditions and real rock heterogeneity, and evaluates the importance of several previously ignored phenomena, e.g., inertial effects and shear-induced motions, thus yielding valuable insight into flow processes at the pore scale in natural rock, and supporting numerical model development and validation.

Rare earth element interactions with UO₂

Rebecca Carter, Ph.D. Candidate

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College of Engineering

Advisor: Amy Hixon, Assistant Professor, Department of Civil and Environmental
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Abstract

Elemental analysis and characterization of surface morphologies and microstructures of nuclear materials have been applied to complement isotopic analysis for both nuclear proliferation and nuclear smuggling activities. Due to interactions with the surrounding environment, samples will age and no longer be in pristine condition. Deciphering the aging processes of complex nuclear materials in various environments is crucial for understanding the changes these materials have experienced from the time of their production and use to the time of sample collection. In particular, studying the diffusion of trace elements into and out of solid-phase nuclear materials in contact with water under different aging scenarios may lead to the identification of definitive aging signatures. As a first step, we used batch sorption experiments to investigate the interactions of twelve REEs (i.e., La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, and Yb) in aqueous solution with uranium dioxide as a function of pH (i.e., 3-9), ionic strength (i.e., 0.025 - 0.5 M), REE concentration (i.e., 100 ppb - 16 ppm), and UO₂ concentration (i.e., 5 - 50 g/L). Aqueous phase concentrations of the REEs were determined using inductively coupled plasma mass spectrometry (ICP-MS) and the morphology of UO₂ was examined using scanning electron microscopy (SEM). Results were in line with typical cation sorption behavior wherein sorption increased with increasing pH and decreased with increasing ionic strength. Preferential sorption of lighter REEs is observed.

Structure-performance relationships and transport mechanisms of charge mosaic membranes

Mark Summe, Ph.D. Candidate

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College of Engineering

Advisor: William Phillip, Associate Professor, Department of Chemical and Biomolecular Engineering

Abstract

Charge mosaic membranes (CMMs) had, until recently, been designed using oppositely charged ion exchange resins (i.e. anionic and cationic) but were difficult to fabricate and properly align. Previous difficulty in processing hindered developments of CMMs. In turn, a fundamental understanding of the structure-property relationship is lacking, which limits the ability to design more effective CMMs. To overcome these difficulties in the fabrication of charge mosaics, our research group recently developed a promising avenue to CMM design by ink-jet printing polymeric materials onto a structural template. Using the striped pattern, positively charged and negatively charged polyelectrolytes are alternatively printed to form the mosaic. We confirmed the presence of these bicontinuous positively-charged and negatively-charged domains by permeating KCl solutions. The CMMs enrich salt, rather than reject, meaning there is a higher concentration of salt in the permeate than in the feed. With a reliable design established, we began to focus on optimizing it by changing processing variables and testing the optimization through transport experiments. Printing of nanomaterials allows for facile design and control over microstructure. The high level of control of processing variables enables a systematic approach to investigate this processing-structure-performance relationship for CMMs. We examined the effect of varying the concentration, molecular weight, and choice of polyelectrolyte as well as the presence of a supporting electrolyte on streaming current and permeability. Printing parameters (e.g. droplet size, distance between drops, and number of layers printed), pore sizes, and structural template allow for greater control over membrane performance. Finally, we sought to elucidate the fundamental transport mechanisms by diffusion, sorption, and filtration experiments with salts of varying concentrations, valencies, and mobilities to isolate entropic and enthalpic contributions. These experiments were facilitated by the unique design of CMM from ink-jet printing with its fine control over the microstructure.

Protection of MoS₂ nanosheets from dissolution by aqueous oxidants using graphitized carbon

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Advisor: Kyle Doudrick, Assistant Professor, Department of Civil and
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Abstract

The unique physicochemical properties of 2D MoS₂ nanosheets makes the material promising for a variety of environmental applications, including photocatalysis, sorption, sensing, and separation. In this study, MoS₂ nanosheets were investigated for their effectiveness as a hydrogenation catalyst for treatment of common drinking water contaminants nitrite and bromate. Hydrothermal synthesis methods were used to synthesis MoS₂ nanosheets of 2H and 1T crystal structure. Synthesized materials were characterized by XPS, XRD, TEM, and Raman spectroscopy. Nitrite hydrogenation activity of the synthesized catalysts, bulk MoS₂ and traditional catalyst Pd/alumina, was evaluated by use of the materials as suspended catalysts in a semi-batch hydrogenation reactor. Concentrations of nitrite and sulfate were monitored during the batch process by ion chromatography. Unexpected removal of nitrite and formation of sulfate (a product of MoS₂ oxidation) in the absence of hydrogen indicated that MoS₂ nanosheets are unstable to chemical dissolution in the presence of aqueous oxidants. Slow dissolution of MoS₂ nanosheets by dissolved O₂ has been demonstrated, but our results show that MoS₂ nanosheets are subject to rapid dissolution in the presence of common aqueous oxidizers. In order to protect MoS₂ nanosheets from chemical dissolution, the particles were coated with a graphitized carbon shell by pyrolysis of a polydopamine shell. Carbon shell thickness was varied by exposure to varying concentrations of dopamine. Aqueous stability and hydrogenation activity of the carbon coated MoS₂ was evaluated by performance as a suspended catalyst in the presence or absence of H₂. Results indicated that carbon coating effectively prevents dissolution of MoS₂ nanosheets even in the presence of aqueous nitrite, however no hydrogenation activity was observed. Alternative applications of the carbon coated MoS₂ were explored including use of the material as a hydrogen evolution reaction (HER) electrocatalyst. Results indicated that thin and intermediate carbon coating did not negatively impact the activity of 2H-MoS₂ nanosheets as an HER catalyst. This study finds that MoS₂ nanosheet instability to aqueous oxidants limits the application of nanostructured MoS₂ to environmental applications and prevents its adoption as a nitrite hydrogenation catalyst. Carbon coating experiments show that protection of MoS₂ can prevent dissolution while maintaining electrochemical properties of the nanosheet.

Catalytic Applications of Bimetallic Ruthenium Molybdenum Phosphide for Selective Furfural Hydrogenation

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College of Engineering

Advisor: Jason Hicks, Associate Professor, Department of Chemical and Biomolecular Engineering

Abstract

Lignocellulosic biomass offers an attractive renewable feedstock for fuels and chemicals. Among the potential feedstock, hemicellulose-derived furfural is a valuable raw material with high market potential. Around 65% of furfural is upgraded into furfuryl alcohol that has various applications in lubricants, resins, fragrances, vitamin C, and lysine production. Due to the reactivity and instability of furfural, many unwanted reactions could occur forming a combination of products from decarboxylation, C=O bond hydrogenolysis, furan rings hydrogenation, and even solvent interactions. These reactivity calls for a catalyst that could perform selective hydrogenation only for aldehyde reduction. Additionally, variety in the functionalities of the feedstock calls for multifunctional catalysts that can withstand this condition.

In this work, bimetallic ruthenium molybdenum phosphide was studied for selective hydrogenation of furfural to furfuryl alcohol. Since furfural is a very reactive component, many other side reactions could occur such as ring hydrogenation and decarbonylation. Therefore, objective of the work is to selectively reduce the C=O in furfural to alcohol and to prevent ring hydrogenation.

Our recent discovery shows that some bimetallic phosphides such as RuMoP are active at low temperature for this aldehyde to alcohol reduction reaction. Our preliminary results show >99% selectivity towards furfuryl alcohol is achievable. The bimetallic effect in RuMoP could be observed in the increased rate constants in comparison to its monometallic analogues MoP, Mo₃P, RuP, and Ru₂P showing bimetallic effect. Moreover, phosphides catalysts showed different catalytic behavior in comparison to reduced Ru metal, in which alcoholic solvents such as isopropanol can interact and produce side products. Interestingly, RuMoP showed preferential ring hydrogenation when electron donating group such as phenol was used, which implied that the electron density of the reactant played an important role in the product selectivity.

The focus of this work is to showcase the ability of metal phosphide to selectively perform hydrogenation reactions in furfural as well as many other functionalities. Additionally, the bimetallic effect observed in RuMoP are studied using a series of kinetic measurements. Finally, the stability of the material was evaluated with a series of catalyst recycling experiments.

A Multi-Level Skew-t Stochastic Generator for Assessing High-Resolution Wind Energy Resources in Saudi Arabia

Dr. Felipe Tagle

Department of Applied and Computational Mathematics and Statistics

College of Science

Advisor: Stefano Castruccio, Assistant Professor, Department of Applied and Computational Mathematics and Statistics

Abstract

Economic and population growth are driving many countries in the Middle East to consider adopting renewable energy sources, such as wind energy, to cope with additional energy demands. Despite its clean and nearly infinite supply, wind energy presents several challenges for integration into traditional energy systems due to its intermittent nature. In this study, we provide a characterization of the wind resource over Saudi Arabia, based on a unique high-resolution weather simulation derived from a state-of-the-art numerical weather prediction model. Furthermore, in order to quantify the uncertainty of the estimates, a stochastic generator of daily wind speed is proposed that allows for the generation of synthetic, spatio-temporally resolved, wind speed time series over said domain. The stochastic generator considers a vector autoregressive structure in time, with innovations from a novel multi-resolution model based on a skew-t distribution with a low-dimensional latent structure. Our results identify regions along the western mountain ranges and central escarpments that are suitable for the deployment of wind energy infrastructure, and establish, based on a conservative wind farm layout assumption, that these regions could potentially provide between 30% and 70% of the national electricity needs.

Thermodynamics and structural complexity of sodium uranyl sulfate minerals with unusual structural topologies

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Advisor: Peter Burns, Henry Massman Professor, Department of Civil and Environmental Engineering and Earth Sciences; Concurrent Professor, Chemistry and Biochemistry

Abstract

Uranium is a critical element with major military and industrial significance. Most uranium minerals are formed because of oxidation-hydration of uraninite¹. The uranyl ion, (UO₂)²⁺, links with various polyatomic anions, such as sulfate, into a wide variety of topologies². Although historically few uranyl sulfates have been described³, within the past decade almost 30 new uranyl sulfates have been described³, with 22 of these new species discovered in the White Canyon mines of southwestern Utah where they primarily occur as efflorescent crusts^{3,4}.

The thermodynamics of the uranyl sulfate group are almost completely unknown¹, perhaps partially due to fundamental limitations in high-temperature calorimetry that have only recently been overcome⁵. Without thermodynamic characterization of mineral phases, predicting the transport of uranium remains difficult. Additionally, certain uranyl sulfates preferentially form over chemically similar minerals in seemingly identical geochemical settings. For instance, péligotite and klaprothite are polymorphs of Na₆(UO₂)(SO₄)₄·4H₂O that share the structural unit [(UO₂)(SO₄)₄]⁶⁻ with several synthetic species⁶. These phases share the same chemistry, but differ in hydration degree, crystal symmetry and crystal complexity, implying underlying subtleties to their formation mechanisms.

This project has undertaken the synthesis, characterization and calorimetric analysis of the White Canyon suite of sodium uranyl sulfates and their closely related synthetic phases. Pure synthetic analogs were crystallized through evaporation in isotherm ovens from solutions of U, Na and S. The crystal structures were solved using single-crystal X-ray diffraction (SC-XRD). The structural complexity of each phase (IG) was calculated using the ToposPro package⁷. The phases were subsequently analyzed with powder X-ray diffraction (PXRD) to verify their bulk purity. Scanning electron microscope (SEM) analysis was also employed to help confirm that each phase is homogeneous. The elemental ratios were verified with inductively coupled plasma optical emission spectroscopy (ICP-OES). The water content was verified with thermogravimetric analysis (TGA). The ground phases were pressed into ~5 mg pellets and dropped into an AlexSys high-temperature 3D Calvet-type calorimeter to measure the heat of dissolution, from which the enthalpy of formation (ΔH_f) was determined.

This project has found that as IG increases, ΔH_f decreases in a linear trend, implying the structural complexity of a phase has an apparent correlation with that phase's stability. As structural complexity has an inverse relationship to configurational entropy⁸, this may imply the formation mechanism of these minerals is energetic rather than entropic. Continuing work will focus on the synthesis of additional sodium uranyl sulfates and the determination of correlations or anti-correlations between complexity and stability.

References (1)J. Plášil. (2014) *J. Geosci.* 59: 99-114. (2)A.J. Lussier et al. (2016) *Can. Mineral.* 54: 177-283. (3)IMA Mineral List Database. Available online: <http://rruff.info/ima/> (accessed 26 February 2017). (4)U. Hålenius et al. (2017) *Eur. J. Mineral.* 29: 1083-1087. (5)A. Navrotsky. (2014) *J. Am. Ceram. Soc.* 97: 3349-3359. (6)A.R. Kampf et al. (2017) *Mineral. Mag.* 81: 753-779. (7)V.A. Blatov et al. (2014) *Cryst. Growth Des.* 14: 3576–3586. (8)S.V. Krivovichev. (2016) *Acta Cryst.* B72: 274-276.

A robust high-sensitivity scanning thermal probe for simultaneous microscale thermal and thermoelectric property mapping

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College of Engineering

Advisor: Yanliang Zhang, Assistant Professor, Department of Aerospace and Mechanical Engineering

Abstract

Scanning thermal microscopy (SThM) is a powerful tool for the characterization of micro- and nanoscale material properties. For instance, SThM can be used as a high resolution and high throughput screening tool for combinatorial materials or nanostructured materials with inhomogeneous properties. Despite their popularity, microscale SThM probes have been demonstrated to simultaneously measure thermal conductivity and thermopower on few thermoelectric materials. Through extensive study we have found that the conventional resistive wire microprobe has several limitations, including high thermal contact resistance, low measurement repeatability and sensitivity, and the inability to establish electrical contact through nanoscale oxide layers. These limitations greatly limit the range of samples that can be measured while the latter renders microscale Seebeck coefficient measurement impossible with traditional sample preparation and handling.

Here we present the development of a scanning thermal probe based on heated resistive wire with novel support structure. The support structure allows unprecedented probe-sample contact force, lowering probe-sample thermal contact resistance, which, in turn, significantly increases thermal measurement sensitivity when compared to the conventional commercial probe. The enhanced thermal sensitivity allows measurement of a wide range of materials with thermal conductivity beyond 20 W/m·K. The higher contact force also grants reliable electrical contact on samples with oxide layers tens of nanometers thick. The spatial resolution of the newly developed probe is experimentally shown to be $\sim 2\ \mu\text{m}$. The probe is demonstrated with quantitative thermal conductivity and Seebeck coefficient mapping on two thermoelectric materials, each with oxide layers up to 25 nm thick: combinatorial Ti-Ni-Sn film and proton-irradiated $\text{Hf}_{0.25}\text{Zr}_{0.75}\text{NiSn}_{0.99}\text{Sb}_{0.01}$. The irradiation-induced change in material properties is reported as a function of depth from the irradiated surface and compared to the vacancy concentration profile derived from theory.

An investigation of the effect of urine compounds on electrochemical oxidation of urea using a nanostructured nickel cobaltite catalyst

Andrew Schranck, Ph.D. Candidate

Department of Civil and Environmental Engineering and Earth Sciences
College of Engineering

Advisor: Kyle Doudrick, Assistant Professor, Department of Civil and
Environmental Engineering and Earth Sciences

Abstract

The effect of urine components on urea electrooxidation using a nickel cobaltite (NiCo₂O₄) electrode in alkaline conditions is presented. Comparison of nickel, cobalt, and nickel cobaltite nanostructures on a carbon paper substrate showed NiCo₂O₄ had the lowest oxidation onset potential (E_{onset}) and optimum current density (J). These results confirmed the ability of cobalt, which is not active for urea electrooxidation, to improve the electroactivity of a NiO electrode. An investigation into electrode substrate selection revealed carbon paper to be a superior material over fluorine doped tin oxide and stainless steel based on geometric electrode area and two benchmarking values: (1) potential at 500 $\mu\text{A}/\text{cm}^2$ (E₅₀₀) and (2) J at 0.65 V (J_{0.65}). The interwoven matrix of the carbon paper promoted greater nanostructured surface area during the hydrothermal synthesis employed. The benchmark data revealed significant impairment for urea electrooxidation in synthetic urine compared to aqueous urea only. In synthetic urine, phosphate, creatinine, and gelatin had the most undesirable impact on electrochemical performance. Further investigation into the binding mechanisms between NiCo₂O₄ and these components was performed using in-situ vibrational spectroscopy. Urea did not strongly interact with the catalyst at pH 13.8, instead interacting through hydrogen bonding or long-range forces. The strong interactions of creatinine with NiCo₂O₄ suggested creatinine blocks urea from interacting with the catalyst when both species are present. While phosphate does not strongly interact with NiCo₂O₄, it may interfere with urea oxidation by either serving as a receptor for urea hydrogen bonding instead of NiCo₂O₄ or blocking urea from interacting with the NiCo₂O₄ surface. While these nanostructured NiCo₂O₄ electrodes show promise for electrolytic urine treatment, minimizing the detrimental effects of the major urine components through improved materials design will be key to achieving economical performance. With continued development, electrolytic cells can be an attractive option for sustainably treating source-separated urine while simultaneously producing hydrogen.

Charge Patterning Affects Ion Transport Through Charge-Mosaic Membranes

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Advisor: William Phillip, Associate Professor, Department of Chemical and Biomolecular Engineering

Abstract

Charge-mosaics, which consist of patterned micro-/nano-scale domains of opposite charge on a single membrane, are capable of transporting ionic solutes more rapidly than neutral particles of comparable or larger sizes. We hypothesize that this unique capability is closely related to the electrostatic interactions between the fixed charge on the membrane surface and the charged solutes permeating through the membrane. Therefore, the proposed study will focus on developing the fundamental knowledge that enables the design and fabrication of high-performance charge-mosaic membranes that can selectively remove salts from aqueous solution by examining these electrostatic interactions in detail. This knowledge will be developed by using our ability to pattern the membrane surface chemistry using inkjet printing devices in order to tailor the membrane surface properties systematically and characterize the corresponding effects on the separation performance. The charge-mosaic membranes present several operational advantages in separation processes where the target solutes are dilute in concentrations (e.g., nutrient recovery from wastewater, recovery of lithium from expired batteries). Therefore, the development of high-performance charge-mosaics through the proposed fundamental studies offers a pathway toward more energy-efficient chemical separations.

Development of a new uraninite reference material for nuclear forensic analysis at high spatial resolution

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Abstract

There is currently a lack of well-characterized matrix-matched uranium-bearing reference materials (RMs) for nuclear forensic analysis at high spatial resolution. To address this deficit, we have characterized a uraninite (UO_2) that can be used as a RM to validate chemical and isotopic signatures in nuclear materials for both the geochemical and nuclear forensics communities. In this study, uraninite from Utah (USA) was identified using powder X-ray diffraction (pXRD) and then characterized for its major, minor, and trace element abundances using a variety of micro-analytical techniques. The chemical signatures of the uraninite were investigated at the macro (cm)-scale with micro-X-ray fluorescence (μXRF) mapping, and at high-spatial resolution (10s of micron-scale) using electron microprobe (EMP) and laser ablation-inductively coupled plasma mass spectrometry (LA-ICP-MS) analyses. Based on EMP analysis, the uraninite is characterized by fairly homogeneous and average contents of 90.37 ± 0.58 % m/m for UO_2 and 2.67 ± 0.13 % m/m for CaO. Due to its homogenous distribution, CaO % m/m abundances were used as the internal standard when conducting LA-ICP-MS analyses in order to calculate trace element abundances and monitor for instrumental drift. Chondrite-normalized rare earth element (REE) abundances show depletion in the light REEs, particularly for lanthanum, with the remaining REEs defining a flat pattern at levels just slightly above 1000 times chondrite. Overall, the major and trace element compositions are fairly homogeneous at both the centimeter and micron scale, allowing this material to be used as a RM for high spatial resolution analysis.

Morphology Dependence of Thermal Conductance in Gold Nanoparticle Systems

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Abstract

Molecular dynamics simulations were performed to model the interfacial thermal conductance from bare gold nanoparticles into a hexane solvent. The computed conductance was found to depend not only on particle shape, but also on the size of the nanoparticles, particularly for nanospheres. These results are compared with conductance out of the planar facets, (111), (100), and (110), which are all commonly exhibited in small patches by the spherical particles.

Undercoordination of the surface atoms and the vibrational density of states in the icosahedra explain some of these observations. The exposed surfaces of icosahedral particles are dominated by (111) facets with 9-coordinated gold atoms. Cuboctahedral particles are dominated by the (100) and (111) facets with 8- and 9-coordinated surface atoms, respectively. The nanospheres approach a constant surface density of 6-9 coordinated sites at large particle sizes, and these surface atoms play a large role in the conductance to the solvent. The surface-normal vibrational densities of states were used to explain a simple surface undercoordination model, which shows a size-dependent enhancement of low-frequency coupling to the solvent.

Functionalized Graphene Enables Highly Efficient Solar Thermal Steam Generation

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Abstract

The ability to efficiently utilize solar thermal energy to enable liquid-to-vapor phase transition has great technological implications for a wide variety of applications, such as water treatment and chemical fractionation. Here, we demonstrate that functionalizing graphene using hydrophilic groups can greatly enhance the solar thermal steam generation efficiency. Our results show that specially functionalized graphene can improve the overall solar-to-vapor efficiency from 38% to 48% at one sun conditions compared to chemically reduced graphene oxide. Our experiments show that such an improvement is a surface effect mainly attributed to the more hydrophilic feature of functionalized graphene, which influences the water meniscus profile at the vapor-liquid interface due to capillary effect. This will lead to thinner water films close to the three-phase contact line, where the water surface temperature is higher since the resistance of thinner water film is smaller, leading to more efficient evaporation. This strategy of functionalizing graphene to make it more hydrophilic can be potentially integrated with the existing macroscopic heat isolation strategies to further improve the overall solar-to-vapor conversion efficiency.

Dissolution of uranium dioxide in uranyl peroxide cluster-forming conditions

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Abstract

Uranyl peroxide clusters exhibiting rich structural diversity have been recently identified as potential candidates for application in an advanced nuclear fuel cycle. Cations present in these systems, typically alkali metals, are essential components, providing charge balance and stabilization of uranyl peroxide building blocks. Herein, we explore the influence of alkali metals in obtaining high concentrations of uranium in solution. We propose that, in the presence of excess hydrogen peroxide, alkali metal concentration governs the solubility of uranium phases by limiting the concentration of uranyl peroxide cluster species that are formed in solution. This hypothesis is applied to uranium dioxide (UO₂), the typical nuclear fuel form, to achieve high solubility (greater than 400,000 ppm U), rivaling the concentrations of uranium yielded by boiling nitric acid dissolution, though in relatively mild, alkaline pH conditions.

Investigation of the Effect of Growth Temperature on Deep Levels in GaAs for Photovoltaics

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Abstract

III-V based multi-junction solar cells have demonstrated the highest photovoltaic conversion efficiencies¹. In these high efficiency multi-junction architectures, a GaAs cell is often selected as the ~1.4 eV absorber. However, the performance of the solar cell can be significantly impacted by the presence of deep level defects, primarily through carrier lifetime reduction. The concentration and type of deep levels that are present in the material is known to vary across growth techniques and with growth conditions², but a clear pattern of how growth parameters affect each level has even now not been fully established. In this study, we use deep level transient spectroscopy (DLTS) to examine the characteristics of deep levels in two n+/p- GaAs sub-cells that are typical of the middle cell in triple-junction solar cells, but grown under different growth conditions. The two samples are grown by metalorganic chemical vapor deposition (MOCVD) at 615 °C and 672 °C. All of the other growth conditions (flow rates, partial pressures, etc.) are maintained the same for both cells. DLTS analysis of the cells reveals the presence of 5 electron traps with activation energies of 0.70 eV, 0.48 eV, 0.52 eV, 0.39 eV, and 0.66 eV in the lower growth temperature GaAs cell, while 4 electron traps, with activation energies of 0.72 eV, 0.57 eV, 0.55 eV, and 0.30 eV, are found in the higher growth temperature junction. The 0.48 eV and the 0.55 eV trap states (in the 615 °C and 672 °C samples, respectively) are likely the same trap level, referred to as EL4² or ET4MO³, which has been reported to arise from interstitial As and antisite defects. A striking dependence on EL4/ET4MO concentration on growth temperature is observed; the 672 °C grown cell has ~38 times larger EL4/ET4MO concentration than does the 615 °C junction. Similarly, the defects with activation energies of 0.52 eV (615 °C) and 0.57 eV (672 °C) show a strong dependence on growth conditions. These states appear to correlate well with previous reports of trap EL3² or ET3MO³. The EL3/ET3MO trap concentration in the 672 °C grown junction is nearly 42 times larger than the concentration in the cell grown at 615 °C. For both of these growth-temperature dependent defect levels, the additional thermal energy during growth appears to be unfavorable for producing solar cells with long minority carrier lifetime. Further investigations are ongoing to validate the physical origins of these defects and to control their formation.

[1] F. Dimroth et al, IEEE Journal of Photovoltaics, vol. 6, (1), pp. 343-349, 2016. [2] G. M. Martin, A. Mitonneau and A. Mircea, Electron. Lett. vol. 13, pp. 191-193, 1977. [3] H. Zhu, Y. Adachi and T. Ikoma, Journal of Crystal Growth, vol. 55, (1), pp. 154-163, 1981.

Synthesis and characterization of new polysulfones containing bulky bridging moieties for gas separation membranes

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Abstract

Polysulfones are widely used polymer membranes for important commercial gas separations due to their excellent thermal and chemical resistance, mechanical stability and ease of synthesis. However, there is significant room for advancement of polysulfone membranes' gas separation performance through innovative molecular design. Here, a series of new polysulfones have been synthesized from a standard diphenylene sulfone with either triptycene and/or phenolphthalein as the bulky bridging unit in the polymer backbone. The composition and chain architecture of this new series of polysulfones were systematically varied to investigate the influence of the rigid, bulky triptycene and phenolphthalein structures on fractional free volume, chain rigidity, and gas transport properties. Incorporation of the triptycene unit provided increased fractional free volume and higher chain rigidity, leading to excellent combinations of permeability and selectivity relative to the phenolphthalein-based polysulfone as well as relevant commercial membranes and previously reported polysulfones. In particular, the triptycene-based polysulfone showed significantly improved selectivities for all gas pairs tested, due to the intrinsic internal free volume of the triptycene unit. For example, the triptycene-based polysulfone displayed an ultrahigh H₂/CH₄ selectivity of 156 and an O₂/N₂ selectivity of 7.7, along with nearly doubled H₂ permeability and ~21% higher O₂ permeability compared to commercial Bis-A polysulfone. Additionally, the triptycene-based polysulfone showed strong resistance to physical aging with little change in performance after 130 days.

Modulation of Charge Recombination in CsPbBr₃ Perovskite Films with Electrochemical Bias

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Abstract

The charging of a mesoscopic TiO₂ layer in a metal halide perovskite solar cell can influence the overall power conversion efficiency. By employing CsPbBr₃ films deposited on a mesoscopic TiO₂ film, we have succeeded in probing the influence of electrochemical bias on the charge carrier recombination process. The transient absorption spectroscopy experiments conducted at different applied potentials indicate a decrease in the charge carrier lifetimes of CsPbBr₃ as we increase the potential from -0.6 to +0.6 V vs Ag/AgCl. The charge carrier lifetime increased upon reversing the applied bias, thus indicating the reversibility of the photoresponse to charging effects. The ultrafast spectroelectrochemical experiments described here offer a convenient approach to probe the charging effects in perovskite solar cells.

DFT and Microkinetic Comparison of Pt, Pd and Rh(111) for Catalytic Ammonia Oxidation

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Abstract

N₂ is the desired product over NO/N₂O for NH₃ oxidation on ammonia slip catalysts (ASC). The selectivity to N₂ of highly active platinum group metals (PGMs), however, are often lower than 80%, insufficient to meet the emission regulations. To date, there is no self-consistent examination of mechanism and selectivity over well-defined PGM catalysts. Here, we perform DFT calculations of all relevant reaction steps in ammonia oxidation on Pt, Pd and Rh (111) and build microkinetic models to predict selectivities at reaction conditions typical of ASC. We show Brønsted–Evans–Polanyi relationships for NH₃ activations by both O and OH. The barriers to oxidative dehydrogenate NH₃ follow Pt < Pd < Rh while they are comparable for surface N₂, NO and N₂O formation. We demonstrate, with microkinetic modeling, that low temperature and deficient oxygen facilitate the formation of N₂ and the selectivity to N₂ follows Pt > Rh > Pd at ASC conditions. The temperature dependence of selectivity is the result of compensation effect, leading to N₂ selective at low temperature and NO selective at high temperature. We demonstrate that the predicted selectivity and overall activation activities agree well with experimental observations. We further perform sensitivity analysis and show that high N* coverage and a lower barrier for N₂ formation than NO/N₂O are key factors to high N₂ selectivity.

Transformation of Uranyl Phosphate and Arsenate Minerals to Soluble Nanoscale Cage Clusters

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Abstract

Understanding the solubility of actinide material in aqueous environments is important in various aspects of the nuclear fuel cycle, including in-situ leaching of uranium ore, reprocessing of spent fuel, determining the behavior of radionuclides in geologic repositories, and the transport of actinide contamination at waste storage sites such as Hanford and at reactor accident sites such as Fukushima. Uranyl minerals with low aqueous solubility, such as uranyl phosphates, vanadates, and silicates, are found as alteration products on tetravalent uranium compounds. Water in contact with these minerals will typically contain much less than 100 ppm of U in solution over a broad range of pH conditions. In the presence of hydrogen peroxide, which is produced by the alpha-radiolysis of water, uranyl minerals and UO_2 readily transform into the water insoluble uranyl peroxide mineral studtite, $[(\text{UO}_2)(\text{O}_2)(\text{H}_2\text{O})_2](\text{H}_2\text{O})_2$.

Nanoscale uranyl peroxide cage clusters (nanoclusters) are hollow cage-like structures made up of 16 – 124 uranyl ions connected by peroxo and hydroxyl bridges. Nanoclusters readily form when studtite and excess hydrogen peroxide are combined in an alkaline environment ($\text{pH} \geq 8$). More than 60 types have been reported with diameters ranging between 1.5 to 4 nm. Many incorporate a variety of bridging ligands and transition metals, including pyrophosphate, oxalate, and nitrate. Uranyl peroxide nanoclusters are generally soluble in water, and solubility measurements of certain clusters have shown uranium concentrations reaching 294,000 ppm U (1.82 M U) in nanocluster-bearing solutions.

This study investigates the reaction of uranyl mineral phases of the meta-autunite group ($\text{An} + [(\text{UO}_2)(\text{PO}_4 / \text{AsO}_4)]\text{H}_2\text{O}_m$) with H_2O_2 -bearing solutions at various pH values containing tetraethyl ammonium hydroxide (TEAOH). A combination of techniques were used to characterize the presence of the mineral studtite and nanoscale clusters in solution. Understanding the transformation of sparingly soluble uranyl mineral phases to highly soluble uranyl peroxide cage clusters and the environmental conditions needed for this transformation can provide insight into potential applications of nanoclusters in the fuel cycle.



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