

Houston Community College and the West Houston Center for Science & Engineering

Presents

The 2016 Research Experiences and Exploration in Materials Science (REEMS) Research Experience for Undergraduates¹

Poster Presentations & Recognition Ceremony



August 16, 2016

Held at Rice University

Bioscience Research Collaborative Building

¹ Funding for this event is provided by the National Science Foundation, Division of Materials Research 1460564 and the West Houston Center for Science and Engineering General Fund. Special thanks to the staff at the Center for Theoretical Biological Physics and the Biosciences Research Collaborative for helping to secure the venue for the REU.

REEMS REU 2016 STUDENTS



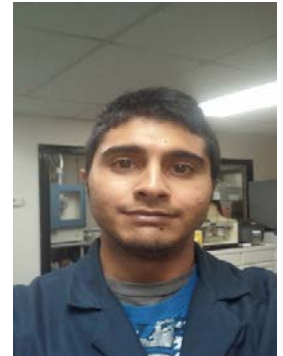
Shams Albayati



Nick Anaya



Eliud Gonzalez-Martinez



Zeshan Rizvi



Niloufar Jafari



Jennifer Pernia



Khoa Pham



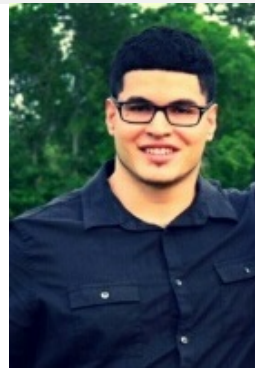
Tammy Hendrix-Doucette



July Romero-Garcia



Grant Foster



Steven Guzman



Raymond McCoy III



Ahmad Sayyedahmad

**The 2016 Research Experiences and Exploration
in Materials Science (REEMS)
Research Experience for Undergraduates**

Poster Presentations & Recognition Ceremony

August 16, 2016

Schedule of Events

<i>8:30 – 9:30 am</i>	<i>Student arrival and poster set-up</i>
<i>9:00 – 9:30 am</i>	<i>Judges Arrive</i>
<i>10:00 – 11:30 am</i>	<i>Poster presenters stand at posters for judging</i>
<i>Noon – 12:45 pm</i>	<i>Lunch</i>
<i>1:00 – 1:45 pm</i>	<i>Poster Awards and Recognition Ceremony</i>

Houston Community College 2016 Summer Undergraduate Research Program in Materials Science

NSF REU: Research Experiences and Exploration in Materials Science (REEMS) for Houston Community College Science and Engineering Students

Bartlett (Bart) M. Sheinberg serves as the Principal Investigator for this award.

The West Houston Center for Science and Engineering (WHC) was awarded funding from the National Science Foundation (NSF) to develop an innovative materials science educational program (REEMS) and a student research program (REEMS REU). The REEMS program and REEMS REU provide a series of multidisciplinary experiences in areas including chemistry, physics, engineering, the biological sciences, medicine, computational science, economics and public policy.

As each student completes their REEMS experiences they are expected to transfer and complete their undergraduate degrees, setting themselves upon a path to exciting academic and professional careers.

Students completing the university physics series, calculus series, and at least one semester of chemistry by the following spring semester will compete to become one of 12 REEMS REU students. Those 12 students that are chosen for the REEMS REU program will participate in summer materials research at Rice University, the University of Houston, and the University of Texas Health Science Center (joining as a REU partner for the 2017 and 2018 summer program).

These activities are funded by an NSF award from the Division of Materials Research No. 1460564



2016 REEMS Research Faculty

Dr. Jakoah Brgoch, Department of Chemistry, University of Houston

<http://jbrgoch.chem.uh.edu/>

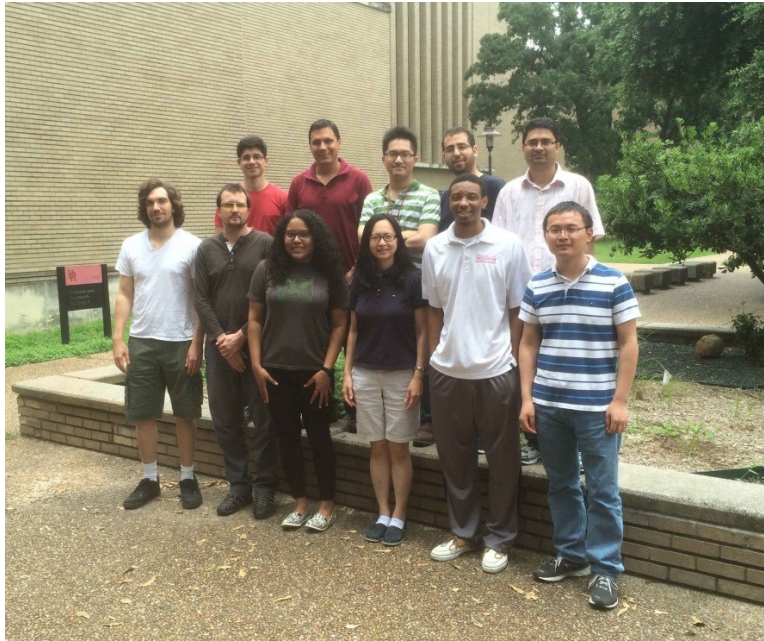
REEMS REU Students: July Romero and Ahmad Sayyedahmad

Students in the Brgoch group are experts in inorganic synthetic chemistry, numerous characterization techniques, and computational chemistry methods. Connecting these research approaches allows the group to solve current problems in a multitude of complex functional inorganic materials.



Front (L-R): Sogol Lotfi, Anna Duke, Erin Finley, Alma Harris, Phu-Cuong Phan, July Romero, Lavanya Kannan. *Back (L-R):* Jakoah Brgoch, Sean Eli, Ahmad Sayyedahmad, Angelica Cobb, Aria Mansouri, Martin Hermus

Dr. Margaret S. Cheung-Wyker, Department of Physics, University of Houston and Center for Theoretical Biological Physics, Rice University
REEMS REU Students: Nick Anaya and Khoa Pham



(Left to right). Front row: Jake, Oleg, Lenaya, Dr. Cheung, Rodney, Pengzhi.
Back row: Andrei, Fabio, Victor, Ezzat, Swarnendu.

Theoretical Biological Physics, Soft Condensed Matter, and Clean Energy

<https://mysm.uh.edu/wiki/projects/cheungroup>

One of the goals of the Cheung group is to discover interesting macromolecular dynamics under cell-like conditions by applying molecular simulation methods. Cellular milieu is a crowded and concentrated environment that impacts the behavior of macromolecules. It can affect the rate of protein folding, protein association, and even the overall conformational changes that cannot be probed in dilute solutions. Examples of the simulation tools used in our investigations include coarse-grained molecular simulation, all-atomistic molecular simulation, and bioinformatic data-mining to investigate the structural behavior and statistical properties of large biomolecules in cellular milieu. To tackle macromolecular dynamics across multiple orders of magnitude in both space and time, we develop a state-of-the-art multi-scale molecular simulation and the utilization of high-performance computing resources to simulate very large systems efficiently.

Dr. James K. Meen, Department of Chemistry and The Texas Center for Superconductivity, University of Houston

<http://www.uh.edu/research/mcf/>

REEMS REU Students: Grant Foster and Jennifer Pernia

Materials Characterization Facility of the University of Houston



The Materials Characterization Facility (MCF) is housed in the Houston's Science Center (HSC) building of the University of Houston's Main Campus. We are part of the [Texas Center for Superconductivity of the University of Houston \(TcSUH\)](#). We specialize in micro-chemical/structural characterization of solid state materials by x-ray and electron beam techniques.

Areas of active research include:

- **Conduct Phase Equilibria Studies on Systems Related to High Temperature Superconductors (HTS) Materials.**
- **Development of High Temperature and High Pressure Experiments for Synthesizing Materials.**
- **Development of the Analytical Capabilities of Electron Beam Instruments.**
- **Conduct Studies in Petrology and Geochemistry (mainly igneous systems)**

Dr. Megan Robertson, Department of Chemical and Biomolecular Engineering, University of Houston <http://jbrgoch.chem.uh.edu/>
REEMS REU Students: Tammy Hendrix-Doucette, Eliud Martinez-Gonzalez and Zeshan Rizvi



**Polymeric Materials
Tailored Structure, Properties, and Function**

The objective of our research group is to develop polymeric materials with enhanced physical properties and function. We specialize in polymer synthetic techniques, structural characterization (small-angle neutron, x-ray and light scattering), thermodynamics and self-assembly, and development of structure-property relationships.

Research projects are focused on the following areas:

Sustainable and biodegradable polymers derived from renewable resources

Advanced materials for wind energy

Structure and dynamics of block copolymer micelles

pH-responsive, antifouling polymer brushes

Multicomponent and multiphase polymer blends

Dr. Rafael Verduzco, Department of Chemical and Biomolecular Engineering, Rice University

<http://verduzcolab.blogs.rice.edu/>

REEMS REU Students: Shams Albayati and Niloufar Jafari

The Verduzco laboratory focuses on the development of complex polymeric materials. We take advantage of advanced polymer synthesis techniques and nanoscale characterization tools to design and characterize polymers at multiple length scales. Current areas of interest include all-conjugated block copolymers for photovoltaics, bottlebrush polymers as responsive surface coatings, liquid crystal elastomers for biomedical applications, and polymers for enhanced oil recovery. The unifying theme of this work is engineering materials at the molecular level to achieve a stronger fundamental understanding of material properties.



Dr. Yan Yao, Department of Electrical and Computer Engineering & Materials Engineering and the Texas Center for Superconductivity, University of Houston

<http://yaoyangroup.com/research>

REEMS REU Students: Steven Guzman and Raymond McCoy III



Yao research group focuses on the materials and devices for energy storage and conversion: understanding the structure-property-performance relationship at the atomic level and designing nanostructured materials for advanced lithium batteries, solar cells, and catalysts. Yao research group was founded on September 2012.

Research Directions:

- **Multivalent Ion Intercalation Materials for High Energy Batteries**
- **Advanced Aqueous Lithium Ion Batteries**
- **All-solid-state Na batteries**

2016 REEMS REU JUDGING PANEL



**Dr. Forrest (Jack) Agee
ADAMCO, Inc.**



**Dr. Allan Jacobson
Texas Center for Superconductivity,
University of Houston**



Dr. Bob Gouchnour
British Petroleum,
Retired



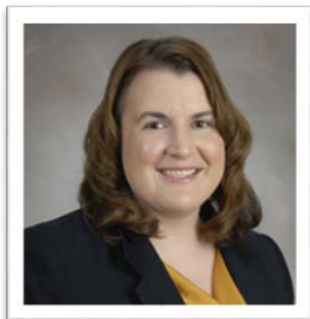
Dr. Carolyn Nichol
Office of STEM Engagement,
Rice University



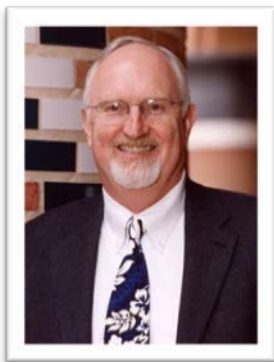
Mr. Zane Marek
District Sales Manager, JEOL USA



Dr. Zachary Cordero
Materials Science and
Nanoengineering, Rice University



**Dr. Laura Smith Callahan
McGovern Medical School,
University of Texas Health
Science Center-Houston**



**Dr. Wade Adams
Materials Science &
Nanoengineering, Rice University**



**Dr. George Stancel
Office of the President
University of Texas Health Science Center- Houston**

2016 REEMS REU POSTER PRESENTERS

<u>STUDENT NAME</u>	<u>EMAIL ADDRESS</u>	<u>FACULTY ADVISOR</u>	<u>POSTER #</u>
July Romero	Alegari3@hotmail.com	Jakoah Brgoch	1
Ahmad Sayyedahmad	Ahmad.sayyedahmad@student.hccs.edu	Jakoah Brgoch	2
Nick Anaya	Naam1595@gmail.com	Margaret Cheung	3
Khoa Pham	Khoa.mpham@gmail.com	Margaret Cheung	4
Grant Foster	grantfoster33@gmail.com	James Meen	5
Jennifer Pernia	Jenniferpernia2011@live.com	James Meen	6
Tammy Hendrix Doucette	thdoucette@gmail.com	Megan Robertson	7
Eliud Gonzales- Martinez	eliud.gonzales@yahoo.com	Megan Robertson	8
Zeshan Rizvi	Zeshan.rizvi@student.hccs.edu	Megan Robertson	9
Shams Albayati	shams.albayati@yahoo.com	Rafael Verduzco	10
Niloufar Jafari	njhsm@yahoo.com	Rafael Verduzco	11
Steven Guzman	stevendguzman@gmail.com	Yan Yao	12
Raymond McCoy III	Rqm3rd@yahoo.com	Yan Yao	13

2016 REU PRESENTER ABSTRACTS

Investigating the Na₂O–SrO–B₂O₃ Phase Space for Potential Rare-earth Phosphors for Use in Solid State White Lighting Devices

Romero J.¹, Anna Duke¹ and Jakoah Brgoch¹

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Solid State Lighting (SSL) is an evolving technology that has the potential to reduce the world's energy consumption. In opposition to the current lighting technologies, it is a reliable source of lighting that is highly efficient and contains materials that are environmentally benign. SSL devices use phosphors to down-convert the blue or UV light emitted by a light emitting diode (LED). The combination of this down-converted light and the LED emission appears as white light. There are certain characteristics that efficient phosphors must have. The optimal phosphor must efficiently down-convert the wavelength of LED emission, be thermally and chemically stable, and have a rigid crystal host structure. Our goal in this research was to investigate the Na₂O–SrO–B₂O₃ phase space for ternary compounds that have not previously been reported as phosphors. Several known compounds were attempted and successfully made through solid-state synthesis. Powder x-ray diffraction, with subsequent refinements, was used to determine compound purity. After extensive analysis of this phase space, a few ternary compounds were singled out as undiscovered potential phosphors. These compounds were then substituted with a small percentage of the rare earth Eu²⁺ or Ce³⁺ to incite luminescence. Luminescent properties of the compounds were examined using steady-state spectroscopy.

This work is supported by National Science Foundation, DMR (1460564)

The effect of vacancies on the electronic and mechanical properties of Zr_3N_4 , Hf_3N_4

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We report a first principle study using density functional theory (DFT) method with the focus on the formation of vacancies in Hf_3N_4 and Zr_3N_4 and their effect on the mechanical properties such as bulk modulus and shear modulus. The optimized lattice parameters show good agreement with the previous theoretical and experimental results indicating the validity of our calculations. With the mean of supercell approach the vacancy formation energy of Hf_3N_4 and Zr_3N_4 is determined to be 2.93 eV and 2.28 eV respectively. Moreover, the vacancy-vacancy formation interactions are determined to be repulsive decreasing the possibility of vacancy clustering. Furthermore, depletion of the mechanical properties of these compounds is observed by increasing vacancy concentrations except for the bulk modulus of Hf_3N_4 which shows an increase at around 6.5 % vacancy concentration. To get more insight, we study the electronic structure of these nitrides with and without vacancies. Both nitrides show small band gaps which is the indication of semiconductors, however after introducing vacancies their density of state (DOS) showed no gap showing metallic behavior. Furthermore, Crystal Orbital Hamilton Population (COHP) calculations show that the dominant bonding in these Th_3P_4 -type structures is the metal-nonmetal bond.

The authors gratefully acknowledge generous financial support provided by the National Science Foundation through No. NSF-CMMI 15-62142)

Exploring the Energy Landscapes of Protein Folding and Electrostatic Effects on Protein Binding Properties

Nick Anaya,^{1,4} Min-Yeh Tsai,^{1,2} Peter G. Wolynes,^{1,2,3}

1. *Center for Theoretical Biological Physics, Rice University, Houston, TX, USA*
2. *Department of Chemistry, Rice University, Houston, TX, USA`*
3. *Physics and Astronomy, Rice University, Houston, TX, USA*
4. *REEMS Program, Houston Community College, Houston, TX, USA*

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Protein folding and binding are two important biological processes that are involved in a variety of cellular functions, such as enzyme activity, signal transduction, transcription regulation, etc. In this study, we employ computational methods to investigate the folding of two globular proteins and the binding properties of two DNA-binding proteins. For the first part, we use a coarse - grained simulation model (AWSEM) to explore the folding energy landscapes of the two proteins: Phase 434 repressor and Ubiquitin. We carry out simulated annealing for these proteins, and monitor their folding trajectories. Our study shows that Phage 434 Repressor folds faster and exhibits less thermal stability than ubiquitin. For the second part, we investigate electrostatic effects on the binding of two dimers (Glucocorticoid Receptor and HU protein) using the Debye-Hückel Potentials in AWSEM. For Glucocorticoid Receptor protein, we examine the binding of the protein dimer using protein frustration analysis. Electrostatic interactions are modeled in order to mimic different solvent dielectric of different solvent media. The results show that Glucocorticoid Receptor experiences a significant increase in frustrated interactions near its Zinc ion binding site when the electrostatic strength is enhanced. This frustration effect prevents the protein from correct binding. For HU Protein, Our results show that the binding of this protein dimer is prohibited. This result suggests that the binding of HU protein requires the presence of its DNA partner in order to achieve correct binding.

This work is supported by the National Science Foundation (PHY-1427654), and the National Science Foundation Division of Materials Research (1460564).

Cooperative DNA binding and deformation by FoxM1 transcription factorsKhoa Pham¹, Davit Potoyan², Peter G. Wolynes²

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2. Center for Theoretical Biological Physics, Rice University

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In the field of cancer biology, intense interest has recently focused on the Forkhead box family (FOX) of transcription factors. FoxM1 (Forkhead box protein M1) is member of the FOX family which is involved in regulating cell cycle and chromosomal segregation. The over expression of FoxM1 is directly linked with common types of cancer in humans as it was observed in the state of uncontrolled cellular growth. FoxM1 has been named molecule of the year 2010 by PDB and is currently being exploited for clinical use as a biomarker for cancer risk prediction, early cancer screening, and molecular diagnostics for further personalized therapeutics. Experimental evidence has shown that FoxM1 is able to “brain wash” normal cells to adopt cancer-like epigenomes. The molecular mechanism via which FoxM1 causes oncogenesis, however remains unknown. Here we use explicit solvent MD simulations to investigate the mechanism by which protein FoxM1 influences the dynamics, and deformation of DNA as well as the cooperative effects of its binding and dissociation. Canonical NPT simulation was used for 1 microsecond to analyze the deformation of FoxM1 to the bound complex. In addition, 1D and 2D umbrella sampling simulation were performed to study the cooperative effect of binding to and dissociation from the DNA. Our results show that FoxM1 deforms the structure of DNA significantly more when acting as dimer than as monomer, increasing the width of major and minor grooves as well as increasing the DNA local axis bending in contiguous base pairs.

This work is supported by the National Science Foundation (PHY-1427654), National Science Foundation Division of Materials Research (1460564)

Alternative Synthetic Routes of Nanocrystalline MoS₂

Foster, G^{1,2}, JK Meen², K Müller²

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Molybdenum disulfide is a semiconductor with unusual electrical properties. Characteristics, such as preferential wavelength absorption and capacitance, are dependent upon grain size of MoS₂ when it is a nanomaterial. MoS₂ is generally made by hydrothermal techniques from organic molecules of molybdenum and sulfur. I investigated whether MoS₂ could be made more simply by mechanochemical synthesis, which is milling together metallic molybdenum and elemental sulfur under ambient conditions. Milling proceeded over 40 days with intermittent sampling of products, characterized by SEM and XRD analysis. SEM showed an intimate mixing of molybdenum and sulfur. Areas dominated by either element became smaller with continued grinding. X-ray diffraction of the starting materials showed peaks for each of molybdenum and orthorhombic sulfur. However, the latter disappeared after the first episode of grinding and were replaced by two broad peaks at relatively low two theta values. These peaks became more pronounced with time of milling. Molybdenum peaks were all maintained throughout the entire milling episode. No Debye broadening of the molybdenum peaks was observed. The two broad peaks could not be assigned to any molybdenum sulfide, polymorph of sulfur, or likely contaminants. Sulfur is amorphized by milling. The products of the reaction between amorphous sulfur and molybdenum could not be identified. Given the increases in intensity of these peaks with milling it is plausible that much extended periods of grinding would yield an identifiable product.

This work is supported by the HCC REEMS Program through the National Science Foundation, DMR (1460564) and grants from the State of Texas to JKM through TcSUH

Possible Use of Calcium Iron Silicate as an electrolyte in a solid oxide fuel cellPernia, J¹, Meen, J.K.², K Müller²

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A solid oxide fuel cell has a reservoir for an oxidizing agent and a reservoir for the fuel separated by a solid barrier composed of two electrodes and an electrolyte. Oxygen molecules are disproportionate on the cathode. Oxygen ions diffuse through the electrolyte to the anode where they react with the fuel, generating electrons. An outside circuit returns the electrons to the cathode. In this way electrical power is generated from the chemical reaction. A perfect electrolyte is strong enough to be thin while being impervious to gas flow and have high oxygen diffusivity. Sclar and Kastelic in 1979 argued for the stability of iron-bearing feldspar at 1200 C. If ferric iron silicates can be synthesized and then the iron reduced without disrupting the crystal structure, silicates with intrinsic oxygen vacancies may be synthesized. The aim of this project was to determine whether calcium ferric iron silicates could be synthesized by crystallization experiments. To this end, a 20 cat. % Ca, 40 cat. % Fe, and 40 cat. % Si oxide bulk composition was prepared by the solid state method. If calcium ferric iron silicates can be synthesized, the next step will be to lower the ambient oxygen pressure. Reduction of the iron to ferrous iron and retention of the crystal structure will necessarily introduce oxygen vacancies to the crystal structure and potentially yield a phase with high oxide ion conductivity. Moreover, the silicate is likely to be a hard crystalline material, if it is similar to its parental compound, plagioclase(anorthite). The bulk composition has hematite (Fe_2O_3), quartz (SiO_2) and a Ca-Fe³⁺-silicate liquid as the super solidus phases. The sub solidus phase assemblage will be described.

Sclar, C.B. and R.L Kastelic (1979) EOS, vol.60, pg 421

This work is supported by the National Science Foundation (CMMI-1334838) and grant from the State of Texas to JKM through TcSUH.

Thermal Analysis of Biorenewable and Degradable Epoxy Resins Derived from Soybean oilHendrix-Doucette, T.;^{1,2} Rizvi, Z.;^{1,2} Gonzales, E.;^{1,2} Yang, G.;¹ Robertson, M.L. ¹Department of Chemical and Biomolecular Engineering, University of Houston, Houston, Texas
REEMS Program, Houston Community College, Houston, Texas

Corresponding author:

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There is a concerted effort to shift our dependence from petroleum based resources to more renewable sources, due to their finite supply and harmful environmental emissions. In addition to supplying energy sources, fossil fuels are dominant sources for polymers and plastics. In this project, vegetable oils are explored as a more sustainable alternative for an important class of polymers: epoxy resins. Epoxy resins are used in a variety of applications such as composites, adhesives, and coatings, and are found in many commercial products as such as in automotive and aerospace industries and structural components. A primary component of epoxy resins is derived from bisphenol A, a petrochemical with known health impacts. The development of biobased alternatives to bisphenol A in epoxy resins will not only contribute to improving the environment but can mitigate potentially damaging health effects. The challenges for developing new materials focus on achieving comparable, or enhanced, physical properties as compared to the conventional materials. In the case of epoxy resins, important physical properties include mechanical and thermal properties. We have synthesized epoxy resins containing epoxidized soybean oil (ESO), to replace the traditional monomer derived from bisphenol A, the diglycidyl ether of bisphenol A (DGEBA). ESO is chosen as a replacement epoxy monomer due to its low cost, biodegradability, sustainable and renewable source and flexible structure which has been shown by other studies to increase the toughness of the epoxy resin. Here, the thermal properties of epoxy resins derived from ESO were investigated by dynamic scanning calorimetry (DSC) to characterize the glass transition temperature. The glass transition temperature defines the transition from the glassy state (an amorphous, rigid solid) at low temperatures (at which the material is typically used in applications) to a rubbery, elastomeric state at elevated temperatures. Polymers were synthesized with varying ratios of ESO to DGEBA, using a curing agent, methylhexahydrophthalic anhydride (MHHPA), to form crosslinked networks catalyzed by 1-methylimidazole. The glass transition temperature of the epoxy resin was found to decrease with increasing ESO content. Epoxy resins with high ESO content exhibited broad glass transitions, in which DSC analysis methods were developed to more accurately characterize the transition temperature. In a targeted range of ESO : DGEBA ratios, two glass transitions temperatures were observed, indicating the presence of phase separated structures. These results indicate the significant impact that the presence of ESO has on the glass transition temperature, a defining characteristic of polymer systems.

This work is supported by the National Science Foundation (DMR-1460564, CMMI-1334838 and DMR-1611376), and Norman Hackerman Advanced Research Program of the Texas Higher Education Coordinating Board (003652-0022-2013)

Hydrolytic Degradation of Biorenewable Epoxy Resins Derived from Soybean Oil and Phenolic Acid

Rizvi, Z.,^{1,2} Gonzalez, E.,^{1,2} Hendrix-Doucette, T.,^{1,2} Yang, G.,¹ Robertson, M.L.¹

Department of Chemical and Biomolecular Engineering, University of Houston, Houston, Texas
REEMS Program, Houston Community College, Houston, Texas

Corresponding author:

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mlrobertson@uh.edu

Biorenewable sources are favorable alternatives to petroleum sources for the synthesis of polymers. Epoxy resins are entrenched in industry as staple materials for use in a manifold array of commercial applications such as aircrafts, automobiles, coatings, adhesives, wind turbines, as well as insulating materials for electrical components. Epoxidized soybean oil (ESO) excels in its abundance and biodegradability to replace traditional petroleum-derived epoxy resins. Epoxy resins derived from ESO and conventional polymer precursors (the diglycidyl ether of bisphenol A [DGEBA] and a curing agent) were synthesized and used in accelerated hydrolytic degradation experiments, at 80°C in a 3 wt% NaOH solution. The degradation was monitored by progressively observing the mass loss over time. Significant differences were observed in the hydrolytic degradation properties of the polymers with varying ESO content. Polymers with 0-40 wt% ESO (relative to the total amount of ESO and DGEBA) displayed little mass loss over 3 weeks (in 3 wt% NaOH solution), while polymers with 60 wt% ESO achieved complete degradation within 2 weeks. Furthermore, polymers with 80-100 wt% ESO displayed complete degradation within 4 days. The addition of ESO provides degradable cleavage points throughout the epoxy resin network structure, allowing for a novel means to recycle or dispose of the polymers after their usable lifetime. The study of ESO-based epoxy resins demonstrates the plausibility of using degradable precursors to synthesize epoxy resins, and was further tested on epoxy resins from a biorenewable source which also provides desirable mechanical and thermal behavior: plant-sourced phenolic acids. This proof-of-concept test on degradable epoxy resins synthesized from renewable sources provides a new outlook on sustainable and recyclable solutions for the perpetual manufacture of these high-demand materials.

This work is supported by the National Science Foundation (CMMI-1334838 and DMR-1611376, National Science Foundation Division of Materials Research (1460564), and the Norman Hackerman Advanced Research Program of the Texas Higher Education Coordinating Board (003652-0022-2013)

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Rizvi, Z.;^{1,2} Gonzalez, E.;^{1,2} Hendrix-Doucette, T.;^{1,2} Yang, G.;¹ Robertson, M.L.¹

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Biorenewable sources are favorable alternatives to petroleum sources for the synthesis of polymers. Epoxy resins are entrenched in industry as staple materials for use in a manifold array of commercial applications such as aircrafts, automobiles, coatings, adhesives, wind turbines, as well as insulating materials for electrical components. Epoxidized soybean oil (ESO) excels in its abundance and biodegradability to replace traditional petroleum-derived epoxy resins. Epoxy resins derived from ESO and conventional polymer precursors (the diglycidyl ether of bisphenol A [DGEBA] and a curing agent) were synthesized and used in accelerated hydrolytic degradation experiments, at 80°C in a 3 wt% NaOH solution. The degradation was monitored by progressively observing the mass loss over time. Significant differences were observed in the hydrolytic degradation properties of the polymers with varying ESO content. Polymers with 0-40 wt% ESO (relative to the total amount of ESO and DGEBA) displayed little mass loss over 3 weeks (in 3 wt% NaOH solution), while polymers with 60 wt% ESO achieved complete degradation within 2 weeks. Furthermore, polymers with 80-100 wt% ESO displayed complete degradation within 4 days. The addition of ESO provides degradable cleavage points throughout the epoxy resin network structure, allowing for a novel means to recycle or dispose of the polymers after their usable lifetime. The study of ESO-based epoxy resins demonstrates the plausibility of using degradable precursors to synthesize epoxy resins, and was further tested on epoxy resins from a biorenewable source which also provides desirable mechanical and thermal behavior: plant-sourced phenolic acids. This proof-of-concept test on degradable epoxy resins synthesized from renewable sources provides a new outlook on sustainable and recyclable solutions for the perpetual manufacture of these high-demand materials.

This work is supported by the National Science Foundation (CMMI-1334838 and DMR-1611376, National Science Foundation Division of Materials Research (1460564), and the Norman Hackerman Advanced Research Program of the Texas Higher Education Coordinating Board (003652-0022-2013)

Designing Ternary Blends of PTB7/PCDTBT/PCBM Solar Cells

Albayati, S.,^{1,2} Jafari, N.,^{1,2} Mok, J. W.;¹ Verduzco, R.¹

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During the recent years, researchers have been trying to find new ways to improve the power conversion efficiencies (PCEs) of the organic photovoltaics (OPVs). The OPVs have demonstrated PCEs above 12% in the recent studies. Current research have demonstrated that conjugated polymers additives can be used to enhance light absorption and facilitate charge separation in polymer/fullerene solar cells. However, there is a lack of understanding in how polymer additives impacts on photoactive layer morphology. The ideal active layer morphology of OPVs plays an important role on the photovoltaic properties of an organic solar cell. The achievement of thermally-stable equilibrium of a donor (PTB7)/ acceptor (PCBM) morphology with continuous inter-penetrable networks, high interfacial areas and nanoscale sized domain can advance the OPVs performance. In this study, we investigate the effect of PCDTBT in PTB7/PCBM solar cells. Here, we designed blends that contain different ratios of the PTB7, PCDTBT and PCBM. The inclusion of PCDTBT improves the photoactive layer morphology and the photovoltaic performance of PTB7/PCBM solar cells. PCDTBT is used as surface compatibilizer modulating the morphology PTB7 and PCBM solar cells to increase the current (J_{sc}) and fill factor (FF) of solar cells. In current work, we are investigating the effect of different ratios of the blends between the PTB7, PCDTBT, and PCBM to produce a more efficient solar cell. Our results so far had shown that adding more PCDTBT to the blends of PTB7 and PCBM is decreasing the current and increasing the voltage. We believe this happened because the ratios are not optimized. Therefore, to improve the solar cell performance we are investigating different ratios of PTB7, PCDTBT and PCBM. In conclusion, controlling the active layer morphology and developing ternary blend can enhance the electronic properties of OPVs solar cells. Therefore, we are developing different compositions of PCDTBT, PTB7, and PCBM to increase the PCEs.

This work is supported by the National Science Foundation (CMMI-1334838 and DMR-1611376, and the National Science Foundation Division of Materials Research (1460564)

Designing Ternary Blends of PTB7/PCDTBT/PCBM Solar CellsAlbayati, S.^{1,2} Jafari, N.^{1,2} Mok, J. W.¹ Verduzco, R.¹

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A polyimide with divalent ion storage capabilities for aqueous-based electrolyte batteries.

Steven Guzman¹, Saman Gheyhani², and Yan Yao²

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Aqueous based electrolytes in batteries has received much attention as an alternative to organic based electrolytes because of the good safety, low cost, good reliability and environmental friendliness in contrast to the dangerous behavior of organic electrolytes presently used in current Li-ion technology. The aqueous electrolyte provides a safe environment in the cell and acts as a good ionic conductor while also absorbing large amounts of heat as a result there exists a good cooling effect in direct contact with both the anode and cathode electrode. However, using water-based electrolyte restrict the working potential of batteries to much lower value while introducing a more challenging system with more side reactions.

In this work, the capabilities of an organic compound for storing different metallic cations from aqueous electrolyte has been investigated. We have focused on an imide-based polymer, Poly-(naphthalene four formyl ethylene diamine (PNFE)). PNFE has already demonstrated a high performance in storage capacity of Li- and Na-ion which introduced PNFE as a good anode material with high capacity and superior cyclability for aqueous Sodium-ion and aqueous Lithium-ion batteries. As a consequence, PNFE electrodes were tested against other divalent and trivalent metal cations. We have demonstrated that PNFE electrode's capability for storing Potassium, Magnesium, Calcium, Zinc, Aluminum and Strontium ions form aqueous-based electrolyte. In addition to its low cost and easy fabrication process, this finding introduces PNFE as a promising material for developing other metal-ion aqueous batteries, and also a good candidate for using in element separation or water purification applications.

This work was supported by the National Science Foundation (DMR-1460564 and CMMI-1400261)

Study of on Hydrogen and Oxygen Evolution in Aqueous Lithium Ion BatteriesRaymond McCoyIII^{1,2}, Saman Gheyhani², and Yan Yao²

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A distinct, and well known, area of energy storage is the battery. In addition to cathodes and anodes, the electrolyte is one of the main components in every battery which conducts an electrical charge between the anode and cathode, in order to produce electrical energy. Presently, lithium-ion (Li-ion) batteries are used in most devices such as cell phones and laptop computers. The electrolyte used in this type of battery is comprised of an organic solvent which is chemically and thermally unstable, as well as toxic. In order to avoid all the issues accompanied with organic electrolytes in Li-ion batteries, an aqueous solution was studied which uses water in place of organic solvents. The problem faced was the potential electrochemical window of water is much narrower, around 1.2V, compared to its organic counterpart which is able to produce up to 5V. At the potential beyond the stable window the process of electrolysis begins to happen, caused by the decomposition of water to oxygen, and hydrogen at high and low potentials, respectively. The effect of electrolyte concentration, and counter ions into the electrolyte, on the potentials where oxygen and hydrogen start to evolve was studied. The experiments were based on the hypothesis that the electrochemical window of water could be increased by adding simpler salt-based ionic compounds at different concentrations. To better understand this process multiple variations of electrolytes were constructed with different salts and concentrations (1molar, 3molar, 5molar, 12.5molar). For each electrolyte, the hydrogen and oxygen potentials were monitored using cyclic voltammetry (CV) tests. Our experimental results set a foundation proving the electrochemical window is able to be manipulated through the changing of concentrations in electrolytes, the use of different salt-based ionic compounds, and application of different metals. Future experiments should produce favorable results if the window is increased, offering a greater option of electrode materials to possibly be used.

This work is supported by the National Science Foundation Division of Materials Research (DMR 1460564), Yao Group & National Science Foundation (CMMI-1400261)

2016 REEMS REU POSTERS

July Romero and Ahmad Sayedahmad
Dr. Jakoah Brgoch, Department of Chemistry, University of Houston



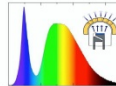
Investigating the Na₂O-SrO-B₂O₃ Phase Space for Potential Rare-earth Phosphors for Use in Solid State White Lighting Devices

July A. Romero, Anna Duke and Jakoah Brgoch
Department of Chemistry, University of Houston, Houston, TX 77204

Introduction to Solid State Lighting (SSL)

Conventional solid state lighting (SSL) devices produce white light by using an inorganic phosphor to down-convert blue or near-UV light produced by a light emitting diode (LED).

The combination of the partial down-conversion and the LED emission is a broad spectrum. Appears as white light.

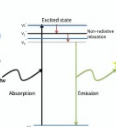


SSL Advantages

- High efficiency
- Small, compact size
- Long device lifetime
- Chemically stable
- Constant environmental performance

Modified Jablonski diagram

Introduce light into the system



The energy is absorbed by the electron, and promotes it to an excited state.

The state wants to lose energy and revert to ground state.

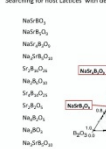
The electron has two main pathways to return to ground state.

The electron can non-radiatively relax to ground state and release energy as heat.

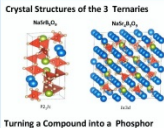
Phosphors release energy by emitting a photon of light.

Na₂O-SrO-B₂O₃ Phase Space

Searching for host lattices with dense crystal structure



Crystal Structures of the 3 Ternaries



Turning a Compound into a Phosphor

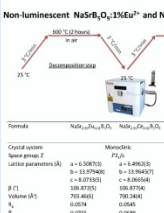
Remove an atom from the crystal structure

Introduce a rare-earth element (e.g. Ce³⁺) to provide luminescence pathway.

Attempted Synthesis of Potential Phosphors

Compound	ZnO ²⁺	ZnO ²⁺	ZnO ²⁺	ZnO ²⁺	ZnO ²⁺ and SrO	ZnO ²⁺ and B ₂ O ₃
Na ₂ O	Phase pure	Phase pure	Phase pure	Phase pure	N/A	Phase pure
Na ₂ SrO	Phase impure	Phase impure	Phase pure	N/A	(100%) Phase pure	N/A

Non-luminescent Na₂Sr₂B₂O₇:2%Ce³⁺ and Na₂Sr₂B₂O₇:1%Ce³⁺

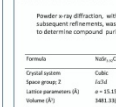


Formula	Na ₂ O ₂ Sr ₂ B ₂ O ₇	Na ₂ O ₂ Sr ₂ B ₂ O ₇
Crystal system	Trigonal	Monoclinic
Space group	R-3m	P2 ₁
Lattice parameters (Å)	a = 0.3087(3) b = 0.3179(4) c = 0.7130(1)	a = 0.490(2) b = 0.304(2) c = 0.605(4)
Volume (Å ³)	108.87(5)	100.07(4)
Z	1	1
Wt %	0.0795	0.0889

Synthesis of Na₂Sr₂B₂O₇:2%Ce³⁺

Polymerizable samples of Na₂Sr₂B₂O₇ were made by grinding stoichiometric amounts of Na₂CO₃, SrCO₃, and B₂O₃. The samples were placed in a furnace under reducing condition at 900°C for 16 hours.

Powder x-ray diffraction, with subsequent refinements, was used to determine compound purity.



Formulas Na₂O₂Sr₂B₂O₇

Crystal system Cubic

Space group Fm-3m

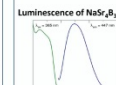
Lattice parameters (Å) a = 0.31106(7)

Volume (Å³) 0.04118(5)

Z 1

Wt % 0.0765

Luminescence of Na₂Sr₂B₂O₇ with Ce³⁺

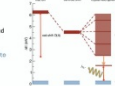


When excited by near-UV light Na₂Sr₂B₂O₇:Ce³⁺ emits in the blue wavelength region.

Not very applicable in the industry

Attempts to red-shift its excitation and emission.

Introduce smaller atoms (e.g. Ca, Li) to increase crystal field splitting.



Conclusions and Future Works

Search the Na₂O-SrO-B₂O₃ phase space and found five potential rare-earth phosphors with three different structure types.

Could make Na₂Sr₂B₂O₇:Ce³⁺ and Na₂Sr₂B₂O₇:Eu²⁺ but need to be refined to show purity.

Made Na₂O₂Sr₂B₂O₇:Ce³⁺ and Na₂O₂Sr₂B₂O₇:Eu²⁺ pure, but they do not luminesce.

Na₂O₂Sr₂B₂O₇ was made pure with Ce³⁺. When excited by near-UV light, it emits blue. Attempts are being made to red-shift Na₂O₂Sr₂B₂O₇:Ce³⁺ excitation and emission, by introducing elements with smaller atoms.


Future work:

Continue to investigate the Na₂O-SrO-B₂O₃ phase space to identify other potential rare-earth phosphors.

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The effect of vacancies on the electronic and mechanical properties of Zr₃N₄ and Hf₃N₄

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Introduction

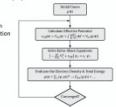
Combining transition metal nitrides with light main group elements (B/C/N) to synthesize super-lattice materials is a considered established approach. Transition metals' high density of d-orbitals allows high compatibility with the s-orbitals of non-transition elements from the closed shell main group elements. Following this approach recently the synthesis of Hf₃N₄ and Zr₃N₄ were achieved using a ball-milled assisted and CVD at high pressure and temperature, up to 18 GPa and 2000 K respectively.¹

Moreover, several metal nitrides are prone to high concentration of point defects, non-metal vacancies specifically. Therefore, we have used density functional theory (DFT) methods to study the effect of vacancies on their mechanical properties.

Density Functional Theory (DFT)

Density functional theory (DFT) is a well-known method to numerically solve Schrödinger equation for many-body system.

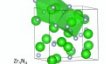
Here VASP software is used with 5-point mesh of Brillouin and PBE functional.



Crystal Structures

Both nitrides have a cubic crystal structure - space group (Fm-3m).

Metals are coordinated by 8 nitrogen (each sharing different coordination).



Vacancy Formation Energies

Vacancy formation energy which by definition is the energy that is required to form a vacancy is calculated using: $E_{vac} = E_{vac} - E_{int} - E_{atom}$

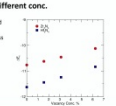
Vacancy formation energies using DFT-C approach to include the relaxation (LLI atoms)

	Zr ₃ N ₄	Hf ₃ N ₄	Zr ₃ N ₄	Hf ₃ N ₄
E_{vac} (eV)	2.79	2.59	2.57	2.57

Reaction formation energies vs different conc.

The reaction formation energies are calculated showing formation energies.

Introducing vacancies makes the formation less favorable.



$3Zr + 2N_2 = HfN_4$

$\Delta E = E_{HfN_4} - 3E_{Zr} - 2E_{N_2}$

$3Zr + 2N_2 = ZrN_4$

$\Delta E = E_{ZrN_4} - 3E_{Zr} - 2E_{N_2}$

Vacancy-Vacancy Interactions

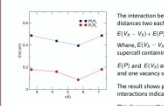
The interaction between two vacancies at various distances from each other is calculated using $E(V_1, V_2) - E(V_1) - E(V_2)$

Where $E(V_1, V_2)$ is the total energy of a supercell containing two vacancies.

$E(V_1)$ and $E(V_2)$ are total energies of perfect and one vacancy supercell.

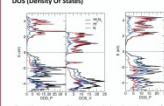
The result shows positive vacancy-vacancy interactions indicating a repulsive interaction.

This decreases the possibility of forming vacancy clusters.



Electronic Structure

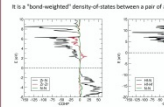
DOS (Density of States)



All nitrides show small band gaps which is the indication of semiconductors introducing vacancies DOS shows no gap showing metallic behavior. The results' behavior might be an error arising from uncorrected local charge within the vacancy. DFT also underestimates the band gap.

COMP: Crystal Orbital Hamilton Population

It is a "bond-weighted" density of states between a pair of adjacent atoms.



For the perfect structure, COMP plots show the non-bonding electrons (on the right side), and the anti-bonding electrons (on the left side). There is almost no bonding between the rare-atom (Zr/Hf) and the non-metal atoms (N) in both cells, and most of the bonding is between the metal and non-metal atoms.

Mechanical Properties

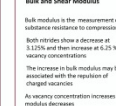
Bulk and Shear Modulus

Bulk modulus is the measurement of the resistance to volume compression.

Both nitrides show a decrease of 3.11% and then increase of 6.2% of vacancy concentration.

The increase in bulk modulus may be associated with the expansion of charged vacancies.

An vacancy concentration increases shear modulus decreases.



Intrinsic Hardness

Experimentally, hardness of a material is measured through an indentation of the surface.

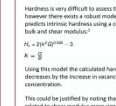
Hardness is very difficult to model theoretically, however there exists a robust model which predicts intrinsic hardness using a combination of bulk and shear modulus.²

$H_v = 2/3(G)^{0.75}(K)^{0.25}$

$K = \frac{E}{1-\nu}$

Using this model the calculated hardness also decreases by the increase in vacancy concentration.

This could be justified by noting that hardness is related to shear modulus more significantly than bulk modulus.



Conclusions

The nitrogen vacancy formation energies of Hf₃N₄ and Zr₃N₄ are reported to be 2.57 eV and 2.57 eV which are lower than HfN and ZrN vacancy formation energy. Showing the higher concentration vacancies.

Density of states (DOS) shows the semiconducting behavior of these nitrides and COMP calculations demonstrated that bonding mainly occurs between Hf or Zr-N.

Bulk modulus shows an initial decrease and then an increase by increasing the concentration of nitrogen vacancies while shear modulus and hardness show constant decrease.

Future Works

Study the charge state of vacancies by adding the correction terms and considering the variation of force level.

Compare bulk properties of Hf₃N₄ and Zr₃N₄ systems to get a better insight of these phase species.

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Nick Anaya and Khoa Pham

Dr. Margaret Cheung, Center for Theoretical Biological Physics, Rice University & Department of Physics, University of Houston



Introduction

Protein folding and binding are two important biological processes that are involved in a variety of cellular functions, such as enzyme activity, signal transduction, transcription regulation, etc. In this study, we employ computational methods to investigate the folding of two globular proteins and the binding properties of two DNA-binding proteins. For the first part, we use a coarse-grained simulation model (AWSEM) to explore the folding energy landscapes of the two proteins: Phage 434 repressor and Ubiquitin. We carry out simulated annealing for these proteins, and compare their folding properties. Our data shows that Phage 434 repressor folds faster and exhibits less thermal stability than ubiquitin. For the second part, we investigate electrostatic effects on the binding of two dimers (Glucocorticoid Receptor and Hb protein) using the Debye-Hückel treatment in AWSEM. For Glucocorticoid Receptor protein, we examine the binding of the protein dimer using protein frustration analysis. Electrostatic interactions are included in order to mimic different solvent densities of different solvent media. The results show that Glucocorticoid Receptor experiences a significant increase in frustrated interactions near its zinc ion binding site when the electrostatic strength is enhanced. This frustration effect prevents the protein from correct binding for Hb protein. Our results show that the binding of this protein dimer is quenched. This result suggests that the binding of Hb protein requires the presence of its DNA partner in order to achieve correct binding.

Methods: AWSEM & DH Potential

Associative memory, Water mediated, Structure and Energy Model

$$V_{DH} = K_{DH} \sum_i \frac{q_i q_j}{\epsilon r_{ij}} e^{-r_{ij}/\lambda_D}$$

Debye-Hückel Potential

$$V_{AWSEM} = V_{WSEM} + V_{DH}$$

(1) Anaya, N., Tsai, M.-Y., Cheung, M., Wolynes, P.G., 2014. J. Chem. Phys. 141, 174701. (2) Anaya, N., Tsai, M.-Y., Cheung, M., Wolynes, P.G., 2014. J. Chem. Phys. 141, 174701. (3) Anaya, N., Tsai, M.-Y., Cheung, M., Wolynes, P.G., 2014. J. Chem. Phys. 141, 174701. (4) Anaya, N., Tsai, M.-Y., Cheung, M., Wolynes, P.G., 2014. J. Chem. Phys. 141, 174701.

Protein Folding

AmcII - Terminal Domain of Phage 434 Repressor (PDB ID: 1469)
 Function: Gene Regulating Protein
 Monomer (α)
 Length: 69 Residues

Ubiquitin (PDB ID: 1ubq)
 Function: Chromosomal Protein
 Monomer (β)
 Length: 76 Residues

Simulated Annealing of Phage 434 Repressor

Structural Analysis of Phage 434 Repressor

Folding Comparison

Conclusion

The results show that Phage 434 Repressor is a fast folder compared with Ubiquitin. Phage 434 Repressor, however, exhibits less thermal stability in experiments.

Protein Binding

Glucocorticoid Receptor with DNA (PDB ID: 1474)
 Function: Transcription Factor
 Chain: A, B (Dimer)
 Length: 77 Residues (Chain A), 77 Residues (Chain B)

Local Frustration Mapped in Structure

Conclusion

The frustration of Glucocorticoid Receptor near its zinc ion binding site increased when electrostatics were added to the simulation. The electrostatic effect is investigated by varying the dielectric constant, mimicking different solvent media.

Ankrahina HD DNA Gyrase Structure (Hb) (PDB ID: 1p71)
 Function: DNA Supercoiling / Negative DNA replication
 Chain: A, B (Dimer)
 Length: 94 Residues (Chain A), 93 Residues (Chain B)

Q Interface

Q Monomer

Conclusion

Ankrahina Hb protein did not find the correct binding position. The Q value generated did not give rise enough to further assist. Therefore further studies are needed in order to know if this particular protein binds with the Hb of DNA.

Acknowledgement

We are grateful to the funding from the National Science Foundation (PHY-1427554), and the National Science Foundation Division of Molecular Research (448046).

Cooperative DNA binding and deformation by FoxM1 transcription factors

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Summary

FoxM1 (Forkhead box protein M1), is a transcription factor, member of the FOX family which is involved in regulating cell cycle and chromosomal segregation. The over expression of FoxM1 is directly linked with common types of cancer in humans. FoxM1 has been named molecule of the year 2010 by PCB and is currently being explored for clinical use as biomarker for cancer risk prediction, early cancer screening and molecular diagnostics for further personalized therapeutics. Experimental evidence has shown that FoxM1 is able to "rewire" normal cells to adopt cancer-like epigenomes. The molecular mechanism via which FoxM1 causes oncogenesis, however remains unknown.

Here we use explicit solvent MD simulations to investigate the mechanism by which protein FoxM1 influences the dynamics and deformation of DNA as well as the cooperative effects of its binding and dissociation.

Molecular dynamics simulations details

We carried out ~1 microsecond long NPT simulation of FoxM1 dimer bound with DNA in explicit solvent and ions.

1D and 2D umbrella sampling simulations were performed to study cooperativity of binding to and dissociation from the DNA. Center of mass distances were used as coordinates for biasing the system. We used 20-50 windows with 2Å spacing for each umbrella window, running 15 ns in each window.

From the umbrella simulations we have mapped out 1D and 2D free energy profiles. From canonical NPT simulation we extracted structural information about the dynamics of DNA deformation in the bound complex.

Free energy profiles of binding

DNA structure deformation deformation by dimeric and monomeric FoxM1

Breaking of base-pairs

Conclusions

- Deforms the structure of DNA: increasing the width of major and minor grooves as well as increasing the DNA axis bending in contiguous base pairs.
- FoxM1 disrupts the base pairing via insertion of its residues deep inside grooves: in several places bases are flipped and make hydrogen bonds with residues of FoxM1 instead of pairing to each other.
- Cooperative effects of binding and deformation of DNA's structure: FoxM1 deforms DNA significantly more when acting as a dimer than as a monomer.


References

Acknowledgments

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Grant Foster and Jennifer Pernia

Dr. James Meen, Department of Chemistry & Texas Center for Superconductivity, University of Houston



Alternative Synthetic Routes of Nanocrystalline MoS₂

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Introduction

What is MoS₂?

- Molybdenum disulfide, in bulk, is an indirect bandgap semiconductor with many promising applications in the fields of catalysis and electronics.
- It has a layered crystal structure like graphite and because of its low friction properties and resistance to corrosion, used in products such as greases, oil and anti-friction lubricant for gears.
- MoS₂ is generally made by hydrothermal techniques from organic molybdates of molybdenum and sulfur.

Background Research


- Currently of great interest in the research of MoS₂ is its electrical properties and the theoretical applications for use in photovoltaic cells, photocatalysis, supercapacitors, and as a catalyst in electrocatalysis processes.
- A recent study of MoS₂ nanoparticles provides a unified explanation of measured photoluminescence spectra as a function of grain size.

Graph showing dependence of the photoluminescence intensity on grain size. The inset shows the experimental setup for the photoluminescence measurement of a single grain of molybdenum disulfide.

- The number of atoms and their distance can be tuned to engineer devices with direct band gaps, allowing an electron to directly emit a photon.

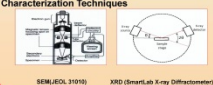
Methods

Preparation



- Phase: 8 g of molybdenum wire and 4 g sulfur into ball mill
- Mill sample for 40 days under ambient conditions
- Intermediate characterization of products

Characterization Techniques




SEM (JEOL 31010) XRD (SmartLab X-ray Diffractometer)

Discussion


SEM showed an intimate mixing of molybdenum and sulfur. Areas dominated by either element became smaller with continued grinding. X-ray diffraction of the starting materials showed peaks for each of molybdenum and orthorhombic sulfur. However, the latter disappeared after the first episode of grinding and were replaced by two broad peaks at relatively low two theta values. These peaks became more pronounced with time of milling. Molybdenum peaks were all maintained throughout the entire milling episode. No delay broadening of the molybdenum peaks was observed. The two broad peaks could not be assigned to any molybdenum sulfide, polymorph of sulfur, or binary compounds. Sulfur is amorphous by milling. The products of the reaction between amorphous sulfur and molybdenum could not be identified. Given the increases in intensity of these peaks with milling it is plausible that much extended periods of grinding would yield an identifiable product.

Results


Week 2



Week 4




Week 6




Backscattered electron images on SEM show progression of sample from distinct elements to an intimate mixing of Mo and S.


Week 0



Week 2 vs Week 4



Week 4 vs Week 6



XRD analysis shows the disappearance of sulfur peaks over time and the formation of two broad peaks of an unknown substance.

Acknowledgements


- This work is supported by the HCC REEMs Program through the National Science Foundation, DMR (140504) and grants from the State of Texas to JFM through TCSUH.
- Special thanks to Dr. James Meen and Dr. Karoline Mueller at Texas Center for Superconductivity at University of Houston.

Objectives

- Study current methods of producing MoS₂ and explore alternative hydrothermal routes.
- Investigate the synthesis of MoS₂ by means of mechanochemistry.
- Understand and employ characterization techniques to analyze samples.


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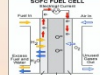


Possible Use of Calcium Iron Silicate as an electrolyte in a solid oxide fuel cell

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Background



What is a solid oxide fuel cell?


Solid-oxide fuel cells (SOFCs) convert chemical energy into electricity more efficiently and with less emissions than conventional generators. Chemical energy may come from reaction of fuel (e.g., natural gas, gasoline, diesel, biogas or hydrogen) with oxygen (air). SOFC generators can power homes, office buildings, and emergency centers worldwide.

What is an electrolyte?

The electrolyte conducts ions between the electrodes, separates the reacting gases and electronically insulates the electrodes, so electrons must flow through an external circuit (Singhal & Kendall, 2001).

Can we make a useful electrolyte from Calcium Iron Silicate?

Scanning Electron Microscope Analysis



The images above were each taken in back scattered electron mode. The gray scale shows differences in average atomic weight. Three crystalline phases are seen – the bright phase is hematite (Fe₂O₃), the dark phase is quartz (SiO₂), the intermediate gray phase is a Ca-Fe silicate. 1150 °C is sub solidus, 1100 °C is super solidus. In the latter case, the gray phase is a glass quenched from a liquid present at 1150 °C and in equilibrium with quartz and hematite. By 1200 °C, a liquid and hematite only coexist. Experiments in which the temperature was raised to 1150 °C were held there for two hours to melt the sample and the sample then cooled to 1130 °C or 1100 °C for crystallization of the liquid. At 1100 °C, there are still large pools of liquid but, at 1150 °C, the liquid has been completely replaced by a mixture dominated by hematite and silicate.

Discussion

Phase relations of CaO-FeO-SiO₂ are known from Osborn and Muan's phase diagram (1965) (LRF). They found extensive solubility of Fe²⁺ in pyroxene and olivine structures. Does the same hold for Fe³⁺? Experiments were performed on 20% CaO, 40% Fe₂O₃, 40% SiO₂ in air. The solidus was determined to be at 1150 °C. An experiment was performed at 1150 °C and then the assemblage cooled to 1100 °C to the liquid crystallized to an assemblage containing Fe³⁺ bearing wollastonite. Further research:

- Are there other ternary Ca-Fe³⁺-silicates?
- Make phase pure samples of each ternary silicate.
- Lower the P(Fe₂O₃) to reduce Fe³⁺ to Fe²⁺.
- Is phase still stable? What is its oxygen content?
- Do oxygen vacancies impart O²⁻ conductivity to this silicate?

Techniques

Sintering

A heat treatment applied to a powder in order to impart strength and integrity. During sintering the atoms in the material diffuse across the boundaries of the particles, fusing together, creating one solid piece. The process is beneath the melting point of material which makes sintering of major use in the shaping process for materials with extremely high melting points.

Quenching

Five samples were placed inside the vertical tube furnace for a measured period at temperatures varying from 1100-1200 °C. A current passed through the hanging wires melts the platinum wire as the sample drops into a quench cup of deionized water. This preserves the high temperature products of reactions so they can be analyzed. This is quenching (rapid cooling of a sample to prevent an unwanted phase change).

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 Houston

Hydrolytic Degradation of Biorenewable Epoxy Resins Derived from Soybean Oil and Phenolic Acid



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Introduction: Societal Need for Biorenewable Epoxy Resins

Motivation:

- Epoxy resins are used in large structural components, coatings, adhesives, aircraft parts, automobile parts, as well as insulation for electrical components
- Petroleum-based epoxy resins do not reasonably degrade after their usable lifetime, and processing of petroleum creates harmful environmental emissions
- The long term sustainability of traditional petroleum-based polymer precursors remains unclear

Research objectives:

- Employ epoxidized soybean oil (ESO) and phenolic acids as alternatives to traditional petroleum-based molecules in epoxy resin applications
- Investigate the accelerated hydrolytic degradation behavior of epoxy resins derived from plant-based molecules which contain ester linkages, anticipated to undergo degradation processes

Advantages of soybean oil and plant-based phenolic acids:

- Abundant sources (including agricultural wastes)
- Biodegradable
- Ester linkages undergo hydrolytic and biodegradation processes
- Non-toxic
- Phenolic acids contain rigid aromatic rings, expected to provide mechanical strength

Synthesis of ESO-Based Epoxy Resins

Epoxy resins were fabricated through the reaction between a multi-functional epoxide-bearing molecule and a multi-functional curing agent.

Protocol A:

- Mix ESO, DGEBA, curing agent, and catalyst at 50 °C for 10 minutes in scintillation vials
- Pour mixture into pan
- Place the mixture in a convection oven at 70 °C for 24 hr, then at 170 °C for 2 hr

Protocol B:

- Mix ESO, DGEBA, curing agent, and catalyst at 50 °C for 10 minutes in round bottom flasks
- Pour mixture into mold
- Place the mixture in a convection oven at 70 °C for 24 hr, then at 170 °C for 2 hr

Characterization of Degradation Rate

- Samples were soaked in a 3 wt% NaOH solution containing 0.04 wt% NaN₃ for varying durations of time
- Samples were then neutralized with a 1 wt% HCl solution, rinsed, and dried overnight in a vacuum oven
- Dry masses were recorded progressively after each degradation period

ESO-Based Epoxy Resins Exhibit Accelerated Degradation Rates

Photos of epoxy resins following soaking in a basic solution for various time intervals:

- Epoxy resin with 100 wt% ESO almost completely degraded after 78 hrs
- Epoxy resin with 0 wt% ESO showed little sign of degradation after 342 hrs

Measurement of mass loss in a basic solution:

- Epoxy resins containing 80 and 100 wt% ESO exhibited rapid mass loss over time in a basic solution, fully degrading in less than 100 h
- Epoxy resin containing 60% ESO exhibited a slower rate of mass loss
- Epoxy resins containing 0-40% ESO did not demonstrate appreciable mass loss

Analysis of degradation rate:

- Linear region was identified in the plot of mass fraction vs. degradation time (in a basic solution)
- Degradation rate was quantified as the slope from the linear fit to the data

Degradable Epoxy Resins from Phenolic Acids with Desirable Mechanical Properties

ESO-based epoxy resins exhibit high degradation rates, yet literature demonstrates their poor mechanical behavior

Phenolic acids contain esters, expected to provide degradability, and also contain rigid aromatic rings, providing desirable mechanical behavior

ESOs based epoxy resins: poor mechanical behavior¹

Phenolic acid-based epoxy resins: desirable mechanical behavior²

Epoxy monomer	Tensile strength (MPa)	Modulus (GPa)
ESA	85 ± 6	3.0 ± 0.3
E4HBA	90 ± 2	2.9 ± 0.2
DGEBA	80 ± 2	2.5 ± 0.2

Hydrolytic degradation of phenolic acid-based epoxy resins:

Monomer	DGEBA	E4HBA	ESA
Degradation rate (mass fraction / h)	3×10^{-4}	6.2×10^{-3}	3.1×10^{-3}

- After 100 h, DGEBA-based epoxy resin shows little mass loss
- E4HBA and ESA-based epoxy resins exhibit considerable mass loss
- Degradation rates of E4HBA and ESA-based epoxy resins are significantly greater than the conventional DGEBA-based epoxy resin

Conclusions


- Significant degradation potential was observed for epoxy resins derived from ESO and phenolic acids
- ESO-based epoxy resins containing 80-100 wt% ESO exhibited accelerated degradation rates compared to the conventional DGEBA-based epoxy resin; the epoxy resins containing 80-100 wt% ESO exhibited 100% mass loss within 100 h of degradation time in a basic medium
- Increasing the soaking time interval increased the degradation rate in ESO-based epoxy resins
- Phenolic acids, also containing ester linkages, provide a route to degradable epoxy resins without loss of desirable thermal and mechanical behavior

Future Work

- Continue degradation experiments on epoxy resins derived from epoxidized salicylic acid and 4-hydroxybenzoic acid
- Study mechanical properties and degradation behavior of other phenolic acid-based epoxy resins
- Explore new methods to ensure better homogeneity in cured epoxy blends of neat DGEBA and ESO

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We thank Brian Rohde, Tyler Cooksey, Vivek Yadav, Wenyeu Ding, Arthur Pratako, and Sharon John (University of Houston) for assistance with experiments and data analysis. We are grateful to Bart Scheinberg, Dr. Chris Christensen, and Dr. Ybran Mercado, and Melissa Ng (Houston Community College) for administering the NSF Research Experiences and Exploration in Materials Science program. We thank the National Science Foundation (CMMI-1334838, DMR-1611376, and DMR-1469564) and Norman Hackerman Advanced Research Program of the Texas Higher Education Coordinating Board (003652-0022-2013) for funding.



Design of Ternary Blend Organic Photovoltaics

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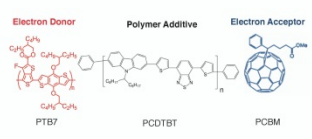
Introduction and Background

Solution-processed organic photovoltaics (OPVs) are attractive as a low-cost and portable source of energy. Comparing to inorganic solar cells, OPVs produce less amount of environmental pollution, are more flexible, lighter, and easier to produce. Conventional OPVs are based on a blend of donor and acceptor semiconductors in the active layer, but recent work has shown that a ternary blend consisting of two donors exhibit superior performance. However, there is poor understanding as to how a third component impacts the active layer morphology and electronic properties. Here, we focused on a ternary blend OPV comprised of two donor polymers (PTB7 and PCDTBT) blended with PCBM acceptor and we explore OPV performance as a function of PCDTBT loading. PCDTBT has a surface energy intermediate to that of PTB7 and PCBM and therefore can act as a compatibilizer. We find that PCDTBT steadily increases the open-circuit voltage and also increases the short-circuit current density at low loadings. The optimal content of PCDTBT was found to be near 20 wt %. Future studies will focus on morphological impact of the PCDTBT additive.

Experimental

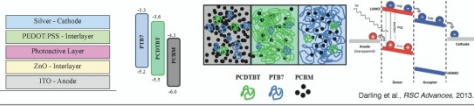
In this study, we focus on a ternary blend of two polymeric donors and an electron acceptor. Specifically, the active layers are comprised of two polymeric donors - poly[N-90-heptadecanyl-2,7-carbazole-alt-5,5-(40,70-di-2-thienyl)-20,10,30-benzothiadiazole] (PCDTBT) and poly(thieno[3,4-b]thiophene-co-benzodithiophene (PTB7) - and a fullerene acceptor phenyl-C61-Butyric acid Methyl ester (PCBM).

PTB7	PCDTBT	PCBM
1	0	1.75
0.9	0.1	1.75
0.8	0.2	1.75
0.7	0.3	1.75
0.6	0.4	1.75
0.5	0.5	1.75
0.4	0.6	1.75
0.3	0.7	1.75
0.2	0.8	1.75
0.1	0.9	1.75
0	1.0	1.75



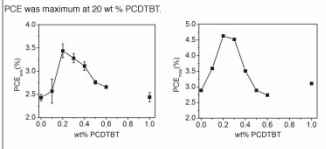
A series of OPV devices were prepared with a varying composition of PTB7 and PCDTBT donors. The relative amount of PCBM was kept constant. The procedure for preparing OPV devices was as follows:

- Clean with Hellmanex, DI water, acetone, and Isopropyl Alcohol (IPA)
- Spin-coat 200 μ L of ZnO solution at 2000 rpm for 1:00 min
- Spin-coat 70 μ L of active layer at 800 rpm for 2:00 min
- Spin-coat 270 μ L of PEDOT:PSS at 5000 rpm for 1:30 min
- Deposit 200 nm Ag

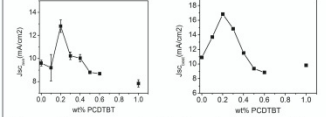


Results

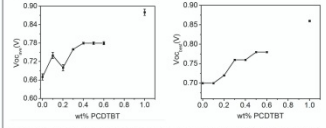
OPVs with systematically varying donor polymer composition were prepared and tested. Below we report the power conversion efficiency (PCE), short-circuit current (J_{sc}), open circuit voltage (V_{oc}) and fill factor (FF) for each active layer composition. The data below show both average and maximum performance for each active layer tested.



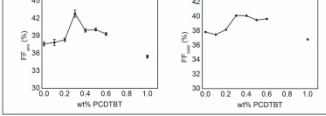
JSC was maximum at 20 % PCDTBT, indicating that the increased current was responsible for the improved performance shown above.



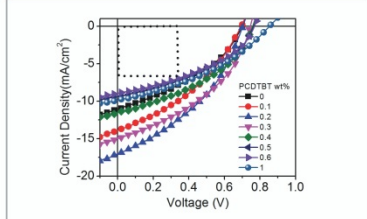
V_{oc} increased gradually and monotonically with increasing PCDTBT content.



The fill factor was relatively constant across the samples tested, and the highest value was found for 30 % PCDTBT.



Conclusions



Our results indicate that ternary blend PTB7/PCDTBT/PCBM OPVs exhibit superior performance compared with either PTB7/PCBM or PCDTBT/PCBM OPVs. We believe that this is due to favorable charge and energy cascading across the PTB7-PCDTBT-PCBM interface. Further work will focus on morphological analysis and comparison with bilayer OPVs. Similar studies will also be conducted on ternary blends of donor and acceptor materials with systematically varying surface energies and compatibilities to understand the relationship of morphology to electronic properties.

Acknowledgements

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A polyimide with divalent ion storage capabilities for aqueous batteries

Battery Set-Up

Coin Cell Components

PNFE Anode Composition

5000x Magnification Electrode

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Electrochemical Reaction

Poly-(naphthalene four formyl ethylene diamine) (PNFE)

a) $\text{PNFE} + \text{Mg}^{2+}, \text{Ca}^{2+}, \text{Sr}^{2+} \rightleftharpoons \text{PNFE}^{\text{Mg}^{2+}, \text{Ca}^{2+}, \text{Sr}^{2+}} + 2e^-$

b) Possible reaction mechanism for PNFE electrode vs divalent ions

Water-based electrolytes restricts the working potential of batteries to a much lower value (1.4V) which introduces a more challenging system with more side reactions

PNFE functions in water based electrolyte but decays in acidic conditions of pH < 2.5

Optimization

Cyclic Voltammetry Testing

Each peak corresponds to a chemical reaction, in this case Magnesium in different concentrations is tested and it was concluded that 2.5 M is the most stable because over 10 cycles there is the least amount of decay

Stable performance of PNFE vs Divalent Ions

Electrochemical charge-discharge performance of the PNFE electrode for different electrolytes containing Mg²⁺, Ca²⁺, and Sr²⁺

Conclusion

An organic anode for divalent ions such as magnesium would allow the creation of new battery chemistries that are potentially safer and cheaper than lithium-based batteries

Acknowledgements

This work was supported by the National Science Foundation (DMT-1460564 and CMMI-1400261), The West Houston Center for Science and Engineering, REEMS Program and the Yao Research Group Energy Materials and Devices

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Study of Hydrogen and Oxygen Evolution Potentials In Aqueous Electrolytes

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Economic Motivation

- Over-consumption of natural resources (petroleum) in today's economy has led to the vast research of cleaner, alternative energies.

	Avg. Oil Consumption (World vs U.S.)
Production	Consumption
World Oil: 31,781,912 bbl/day	18,078,486 bbl/day
U.S.: 4,815,395 bbl/day	8,678,045 bbl/day
	2,538,650 bbl/day

Hydrogen and Oxygen Evolution Potential Methods

Hydrogen and oxygen evolution is a process caused by electrolysis. When a direct electrical current (DC) is applied to an aqueous electrolyte, as it becomes unstable, it breaks the bond between the H₂O and simultaneously produces hydrogen and oxygen gas.

Flooded Cell

Cyclic Voltammetry (CV) Testing

Hydrogen & Oxygen Evolution (Full Cycle Windows)

Research Solution

- Increase the electrochemical window of aqueous electrolytes by monitoring the hydrogen and oxygen evolution potential in order to manipulate its origin with simpler salt-based ionic compounds.

Real-World Application

- Lithium-ion batteries are the dominant energy source for today's electronics; using organic solvents as the preferred electrolyte to dissolve complex ionic compounds and produce an electrical charge.

Electric Car

Electrochemical Window

- Due to the chemical and thermal instability of organic solvents used in electrolytes, water is used in its place
- The electrochemical window of water is around 1.23V
- Organic electrolytes are able to reach up to 5V
- The window is able to be widened with different concentrations of salt-based ionic compounds

Cathode & Anode Materials Dictated by Window

Results

- With the application of a stable electrolyte, and corresponding active materials of lithium manganese-oxide and PNDE, the completed flooded cell was able to reach 140 mA/h at 1.8V

Conclusion

Our experimental results set a foundation showing the electrochemical window of water is able to be manipulated through the changing of concentrations in electrolytes, the use of different salt-based ionic compounds, and application of different metals. More in-depth research should increase the window, offering a greater option of electrode materials to possibly be used.

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