



March 30 – April 1, 2023 @Texas State University Campus

CONFERENCE PROGRAM AND ABSTRACT BOOKLET





The University of Texas at Austin Center for Dynamics and Control of Materials



materials research science

engineering center









LBJ GRAND BALLROOM • SAN MARCOS, TX



Thursday, March 30 LBJ Student Center Grand Ballroom

Start Time	Description
6:00 pm	Kick off ceremony & welcome dinner

Friday, March 31 LBJ Student Center Grand Ballroom

Start Time	Description
8:30 am	Continental Breakfast and registration
9:00 am	Introduction to Texas PREMs
10:00 am	PREM Alum: Carlos Corona, CEO Southwest Yeast Lab LLC
10:30 am	PREM Alum: Dr. Mirella Vargas, Southwest Research Institute
11:00 am	Social
11:20 am	PREM Alum: Mauricio de Leo, Ph.D. Student University of Minnesota
11:50 am	MRSEC Alum: Dr. Manuel Dominguez, 3M
12:20 pm	Lunch
1:20 pm	Oral presentations by PREM students
2:30 pm	Entrepreneurship workshop facilitated by Dr. Harlan Beverly, VP of Engineering, Mercado Labs and Lecturer in Entrepreneurship and Innovation at Texas State University
4:30 pm	Poster session & networking
6:00 pm	Dinner





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Saturday, April 1 RFM Lobby (@ 9 am) and RFM 3224 (@ 10:30 am)

Start Time	Description
8:30 am	Continental breakfast
9:00 am	Laboratory/facility tours
10:30 am	Presentation and poster awards
11:00 am	Student reflections on PREM
11:45 am	Closing remarks





March 30 – April 1, 2023 @Texas State University Campus

INVITED SPEAKERS

LBJ GRAND BALLROOM • SAN MARCOS, TX



Carlos Corona CEO Southwest Yeast Lab

Affiliation Texas State PREM Alum

Carlos Corona has 8 years of research experience in chemistry, biochemistry, physics, and psychology. His real passion is where business and science intersect which led him to study chemistry, leadership, business management, communication, and psychology at Texas State University. After graduating in 2019, he worked in the startup arena to develop a sustainable, biochemical nanotechnology from lab to commercialization for the company, Nabaco, located in Central Texas. After raising \$1.5M and leading as Director of Technology for the Txstate startup, he founded Southwest Yeast Lab LLC in 2021 and now serves as the CEO for the company.



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2023 Texas PREM Conference



Mirella Vargas, Ph.D., P.E. Senior Research Engineer Southwest Research Institute UTEP PREM Alum

Dr. Vargas is a senior research engineer in the Materials Science and Failure Analysis Group at Southwest Research Institute (SwRI). Dr. Vargas supports and conducts failure analysis and applied research projects involving, metals, advanced materials, and coatings in diverse applications using a wide range of materials and chemical characterization tools.

Dr. Vargas previously worked at the NAVAIR Fleet Readiness Center Southeast supporting the repair and overhaul of NAVY based aircraft and weapon systems. Dr. Vargas conducted various metallurgical failure analyses on structural airframe and engine components, and provided manufacturing instructions for flight critical components.

During her graduate work at The University of Texas at El Paso (UTEP), Dr. Vargas focused on the fabrication and characterization of nanostructured thin films for

optoelectronic and photovoltaic device applications. Dr. Vargas worked transition metal oxide thin films fabricated by physical vapor deposition techniques- including radio frequency (rf) and direct current (dc) magnetron sputtering. The deposition parameters were varied to ultimately tailor the visible absorption of the films in order to exhibit a high transparency and critical conductivity for application as transparent conducting oxides. Dr. Vargas published various articles on the structure-function properties developed by variable deposition parameters on tungsten and titanium oxide thin films.



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2023 Texas PREM Conference



Mauricio De Leo Materials Science Ph.D. Student University of Minnesota University of Texas Rio Grande Valley PREM Alumni

Mauricio De Leo is a *Chemical Engineering and Materials Science* (CEMS) doctoral student and Frank Snowden fellow at University of Minnesota (UMN) in Prof. Nathan Mara's research group. His research interests focus on enhancing the mechanical performance of materials by understanding the fundamental role of metal interfaces and defect-interface interactions at the nanoscale.

Mauricio received a BSc in Physics and a BSc in Chemistry and a minor in Business Administration from the University of Texas Rio Grande Valley. Before joining the CEMS department at UMN, he worked as an undergraduate research



assistant in the Advanced Nanoscience Laboratory under the tutelage of Dr. Karen Martirosyan, working on microfluidics, magnetic particle synthesis for cancer theranostics, magnetoelectric material research, and magnetic membranes technology. Recently, along with his business partner Zachary McAllister, Mauricio won the 2023 CEMS Crucible Award in a business pitch competition with their company "*Greener Forward: A sustainable energy storage solution*".

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2023 Texas PREM Conference



Manuel N. Dominguez Sr. Regulatory Affairs Engineer 3M Company UT Austin MRSEC Alum

Speaker Bio

Manuel Dominguez is a Sr. Regulatory Affairs Engineer working for the Transportation Safety Division of the 3M Company. Manuel is responsible for improving safety and standards globally for roadways and vehicles. Manuel received his Ph.D. at the University of Texas at Austin in 2022 in chemistry while conducting research for Prof. Delia Milliron on nanomaterials, nano-assembly and their optical properties. He was a MRSEC Alum from UT Austin and an NSF Fellow. He received his B.S. in chemistry from the University of South Carolina in Aiken and was a Magellan and ACS Scholar. Prior to pursuing his education, he served in the United States Military.











Harlan T. Beverly, Ph.D. VP of Engineering, Mercado Labs

Lecturer in Entrepreneurship and Innovation, Texas State University

Harlan T. Beverly, Ph.D. is a 4-time CEO and 3-time startup founder with special focus in the web technology space (B2B and B2C). He is currently VP of Engineering at a startup (Mercado Labs) and a lecturer in entrepreneurship and innovation at Texas State University. Harlan is also a mentor and advisor in dozens of startups at Capital Factory and NewChip. Harlan has 21 published technology patents and numerous scholarly articles as well as two published books: <u>https://amzn.to/377aR3b</u>. Previously, Harlan was a lecturer at The University of Texas at Austin where he taught entrepreneurship and helped run the

Texas Venture Labs. Harlan specializes in fundraising and growth marketing for consumer, health, and technology companies. Harlan has founded three B2C startups and sold two of them: Bigfoot Networks, Inc. and Karmaback, Inc. Harlan was also CEO of Key Ingredient, Inc. which he sold in 2018. Harlan is not actively investing but has experience as an angel investor and a venture investor and is an active mentor at Capital Factory in Austin, TX. He received his B.S. Electrical in from Ohio Northern Engineering M.B.A. University, an from The University of Texas at Austin, and his PhD in Business from Oklahoma State University.











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STUDENT ORAL PRESENTATIONS

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Quantum effects in the electronic properties of epitaxial SrTiO₃ films on Si(001)

Barry Koehne^{1,2}, Dr. Ryan Cottier³, John Miracle^{1,2}, Dr. Nikoleta Theodoropoulou^{1,2} ¹Materials Science Engineering and Commercialization Program, Texas State University ²Department of Physics, Texas State University ³Teledyne Inc.

Abstract

We investigate the electronic properties of epitaxial SrTiO₃ films on p-Si(001) using lowtemperature magnetotransport measurements. We show that the temperature and magnetic field dependence of the conductivity can be entirely determined by 2D quantum corrections due to quantum interference and electron-electron interaction effects. For low carrier concentrations <10¹³ cm⁻² epitaxial strain seems to strengthen electron-electron interactions while at higher electron concentrations >10¹⁴ cm⁻² spin-orbit coupling dominates. While for both low and high electron concentrations we observe single-carrier transport, at intermediate electron densities ~10¹³ cm⁻² (near the Lifshitz transition point) and below 40 K , two-carrier transport is evident by a non-linearity of the Hall resistance. X-ray Photoemission Spectroscopy depth profiling show consistent elemental ratio throughout the film with a change in oxidation states near the Si interface. The change in oxidation state indicates the presence of a larger amount of oxygen vacancies near the interface. SrTiO₃ is grown coherently on Si(001) by a 45° rotation around the surface normal using Oxide Molecular Beam Epitaxy (MBE) at low Oxygen pressures to avoid formation of SiO₂ at the interface. X-ray diffraction phi and survey scans and x-ray reflectivity scans show that SrTiO₃ is single crystal and that the interface between Si and SrTiO3 is abrupt.

This work was supported in part by the NSF Career Award DMR # 1255629, a Partnership for Research and Education in Materials (PREM) NSF Grant DMR-2122041, DoD grant 78810-W911NF-21-1-0253, and the National High Magnetic Field Laboratory. The National High Magnetic Field Laboratory is supported by NSF through NSF/DMR-1157490/1644779 and the State of Florida.

Biography of Presenter

Barry Dean Koehne obtained his Bachelor of Science in Physics (2015), Master of Science in Physics (2018) from Texas State University. He is currently working on his Ph. D. in Material Science Engineering and Commercialization (MSEC) at Texas State University. He has presented at conferences such as the international workshop on Oxide electronics and APS. He has been trained and has performed experiments at the National High Magnetic Field Laboratory in Tallahassee, Florida.







Liquid Azobenzene: Applications in Solar Energy Storage and Reversible Adhesives

Scott Barrett,¹ Jacob Guerrero, Makena Burns and William J. Brittain¹.

¹Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX 78666

Abstract

Solar thermal fuels are compounds that store solar photon energy by photoisomerization to a higher energy, metastable state. Azobenzene is one potential photoswitch for solar thermal fuels and has advantages of photostability and facile synthesis. Subsequent release of heat can occur spontaneously or by visible irradiation. The *cis-trans* isomerization is the energy storage process for azobenzene. Substituents can control irradiation wavelength, lifetime of metastable stable state, and isomerization enthalpy (Δ H=150-

300 J/g). If one envisions a solar energy storage system that utilizes flow between the solar collection and heat exchanger, then azobenzenes with *cis* and *trans* melting points above the operating temperature would enable flow technology. Our strategy for synthesizing and characterizing energy storage azobenzenes is guided by a comprehensive literature survey of azobenzene melting points. Generally, *cis* melts lower than *trans* due to more disordered structure. Because the azo bond is the locus of energy storage, adding substituents will reduce the gravimetric energy density. Therefore, our initial studies focus on mono-substituted azobenzenes. For the same substituent, the melting points increase in the order *para > meta > ortho*. The most promising substituents are methyl, ethyl, methoxy, trifluoromethyl, and fluoro. These functional groups are afforded from a facile synthetic schema with efficient and fast reactions. We report our initial data on fluoroazobenzene where the compounds were characterized by UV-Vis, NMR, and differential scanning calorimetry.

Biography of Presenter (in 11 Pt Arial Font)

Scott Barrett is a Graduate Research Assistant at Texas State University. He received his B.S.

of Chemistry from Texas State University in 2017 and M.S. of Chemistry in fall of 2022. He is currently in the MSEC (Material Science, Engineering, and Commercialization) PhD program at Texas State University. He practices synthetic organic chemistry over photochemical species such as Azobenzene and Spiropyran. Currently his research focuses on solar fuel cell functionalization with a specialty in Azobenzene synthesis. He is interested in researching other organic chemicals for material science applications into renewable energies, such as solar panels.







Quantum Well Mediated Sub-Thermal Electron Injection to Silicon at Room Temperature

Anthony Martinez,¹ Pushkar K. Gothe,¹ Ojas T. Bhayde,¹ J. Tyler Gish,² Vinod Kumar Sangwan,² M. R. Tiscareno,¹ Thevnin Rumende,¹ Michael P. Rabel,¹ Gumaro Garcia Gonzalez,¹ Adrian Gomez,¹ Jiechao Jiang,¹ Yi-De Liou,¹ Ye Cao,¹ Efstathios Meletis,¹ Mark C. Hersam,² Seong Jin Koh¹ ¹The University of Texas at Arlington, Arlington, Texas 76019 ²Northwestern University, Evanston, Illinois 60208

Abstract

At room temperature, electrons in solids are thermally excited following the Fermi-Dirac distribution. While this electron thermal smearing is a natural thermodynamic phenomenon, it leads to many unwanted characteristics in electronic and spintronic devices. For example, the electron thermal smearing is the root cause of the excessive heat generation (or power consumption) in the most advanced transistors in laptops, tablets, and data centers. Here we present an approach in which transport of thermally excited electrons is selectively blocked and only non-excited electrons (cold electrons) are allowed to participate in electron transport at room temperature. This is realized by employing a quantum well (QW), whose discrete energy state filters out thermally exited electrons. Our model device consists of source electrode (Cr), tunneling barrier 1 (1-2 nm Al₂O₃ or Cr₂O₃ layer), QW (3-5 nm SnO₂), tunneling barrier 2 (2nm SiO₂), and p-type Si, where electrons tunnel from the source to QW, and then from QW to Si. The filtering of thermally excited electrons by the QW state is demonstrated through current-voltage (I-V) measurements of the fabricated devices, which show abrupt current jumps and extremely narrow widths of the corresponding differential conductance (dl/dV) peaks. The full width at half maximum (FWHM) of the differential conductance peaks was measured to be as small as 0.25 mV at room temperature, which corresponds to an effective electron temperature of 0.8 Kelvin. This energyfiltered sub-thermal electron transport may find important applications in many electronic and spintronic devices whose performances are degraded due to electron thermal smearing. If it is implemented into transistor architecture, for example, it could produce energy-efficient electronic devices that can operate with extremely-low power consumption at room temperature. This work was supported by the National Science Foundation (DMR-2122128, DMR-1720139, and ECCS-2031770).

Biography of Presenter

Anthony Martinez is a Ph.D. student at The University of Texas at Arlington. He got his B.S. in Physics and Mathematics at the University of Houston. He has presented his Ph.D. research at several meetings and conferences like 2022 MRS Fall Meeting and Exhibit at Boston. At UTA, he is part of the prestigious engineering society, Tau Beta Pi.





Pulsed Laser Deposition of Vertically Aligned β Ga2-xWxO3 Nanocomposites for Self-Biased Solar-Blind Ultraviolet Photodetectors

<u>Francelia Sanchez Escobar</u>^{1,2}, Debabrata Das^{1,3}, C. V. Ramana^{1,3} ¹Center for Advanced Materials Research (CMR), University of Texas at El Paso, 500 W University Ave, El Paso, Texas 79968, USA ²Department of Metallurgical, Materials, and Biomaterials Engineering, University of Texas at El Paso, 500 W University Ave, El Paso, Texas 79968, USA ³Department of Aerospace and Mechanical Engineering, University of Texas at El Paso, 500 W University Ave, El Paso, Texas 79968, USA

Abstract

The energy consumption has increased over the last decades due to the technological advancements which require high energy-efficient multifunctional devices. Self-assembled vertically aligned β-Ga2-xWxO3 nanocomposite (GWO-VAN) architecture were grown on silicon platform by pulsed laser deposition for the application in low-cost self-biased solar-blind UV photodetector. The W-enriched vertical β Ga2-xWxO3 nanocolumns inside the W-deficient β-Ga2-xWxO3 matrix were fabricated by controlling the growth parameters. The presence of β-Ga2xWxO3 was confirmed from structural and morphological characterization using x-ray diffraction, HAADF-STEM and probe tomography. x-ray spectroscopy, atom Furthermore, photoluminescence spectroscopy assisted to understand the dynamics of photo-absorption and the recombination between energy states. Cost-effective MSM-type UV PD was fabricated using β-Ga2-xWxO3 VAN as the active material with a silver top metal contact. The device was characterized to test its responsivity, detectivity, among other measurements.

Biography of Presenter (in 11 Pt Arial Font)

Francelia Sanchez is a third year PhD student in materials science and engineering at the University of Texas at El Paso. She has a bachelor's degree in metallurgical and materials science and engineering. Francelia has enjoyed doing research since her senior year. Her current research explores the pulsed laser deposition of the ultra-wide band gap semiconductor, gallium oxide.





Anisotropic Two-photon Excited Photoluminescence of InGaN Nanowires

<u>Emma M. Sundin</u>^{1,2}, Debabrata Das^{2,3}, Kausik Kolluri⁴, Pallab Bhattacharya⁵, C.V. Ramana^{2,3}, Chunqiang Li⁶

 ¹Department of Metallurgical, Materials and Biomedical Engineering, University of Texas at El Paso, El Paso, TX, USA
²Center for Advanced Materials Research (CMR), University of Texas at El Paso, El Paso, TX, USA
³Department of Aerospace & Mechanical Engineering, University of Texas at El Paso, El Paso, TX, USA
⁴Department of Physics, University of California Santa Barbara, Santa Barbara, CA, USA
⁵Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI, USA
⁶Department of Physics, University of Texas at El Paso, El Paso, TX, USA

Abstract

Gallium nitride (GaN) and its derivatives are important materials for optoelectronic and electronic applications such as light emitting diodes, solid state lasers, optical modulator, and artificial photosynthesis. The controlled growth and manipulation of these materials at the nanoscale and an understanding of their linear and nonlinear optical properties lay the foundation for developing next-generation optoelectronic and electronic devices. In this context, we report the two-photon absorption and anisotropic two-photon excited photoluminescence observed in indium gallium nitride (IGN) nanowires grown by molecular beam epitaxy. The IGN nanowires were imaged using a house-built two-photon photoluminescence microscope with a tunable femtosecond laser to excite over the near-IR range (690-950 nm). In addition, to explore the polarization response of this material, the polarization angle of the excitation electric field was rotated, and emitted photoluminescence was analyzed with a polarizer. Results show polarized photoluminescence with a stronger signal in the direction perpendicular to the IGN nanowires' axis. Also, we observed strong two-photon absorption above the bandgap, with several excitation spectrum peaks near 740, 790, and 870 nm. These peaks showed an anisotropic response to the excitation polarization angle, which may be due to the anisotropy of IGN nanowire's wurtzite phase. The polarizationdependent properties of light absorption and emission reported here for IGN nanowires may be useful in optimizing these materials for future optoelectronic device applications.

Biography of Presenter

Emma Sundin completed a BS and MS in Physics before pursuing a PhD in Biomedical Engineering. Her work has included research in optical properties of semiconductor materials as well as non-diffracting optical beams for microscopy applications.





Understanding polymer shear profiles when processed by Micro-Compounders

<u>Narcedalia Anaya Barbosa</u>,¹ Joshua Goetz², Christopher J. Ellison, Frank S. Bates ¹Author's affiliation: University of Minnesota ²Author's affiliation: University of Texas Rio Grande Valley

Abstract

This research provides a better understanding of the rheological behavior of polyethylene at different processing conditions using the DSM Xplore 5 and 15 cc micro-compounders. Polymers used were high density polyethylene (HDPE) with a linear architecture, low density polyethylene (LDPE) showcasing a long chain branched structure, and linear low density polyethylene (LLDPE) exhibiting a short chain branched architecture. Measurements obtained in the micro-compounders were compared to those obtained with an ARES-G2 rheometer for a range of shear rates (50, 100, 150, 200 and 250 RPM), temperatures (150oC, 200oC), fill volumes (80%, 90%, 100%) and polymers. The measurements were used to evaluate the accuracy of the micro-compounders and scalability between the systems. Comparing the rheometer data and micro-compounder predictions can aid in identifying differences related to the polymer architecture and help to understand the impact of simple and extensional shear on the polymer when it is processed. **UTRGV_Anaya Barbosa_Narcedalia_Abstract**.

Abstracts are due March 8 at 5 pm and are to be submitted in both PDF and WORD format to this folder: <u>https://securetransfer.txstate.edu/filedrop/COSE-CHEM-prem_conference</u> These files will be compiled and distributed electronically to all conference participants.

Biography of Presenter

Chemistry student and PREM undergraduate researcher at UTRGV with two years of studies in nanotechnology, and three years of experience in laboratory research.



Role of Solvent Composition During Processing of Stimuli-Responsive PNIPAM/Silyl Methacrylate Copolymers

<u>Fabian A. Rodriguez</u>,¹ Jason D. Linn,² Diana Y. Zhang,² Michelle A. Calabrese,² ¹Author's affiliation: University of Texas Rio Grande Valley ²Author's affiliation: University of Minnesota

Abstract

In this study, poly(N-isopropylacrylamide-co-3(trimethoxysilyl)propyl methacrylate copolymer (PNIPAM -co-TMA) has been studied as thermal-responsive glass coatings due to optical properties stemming from thermally reversible phase changes. These phase changes result from the abrupt coil-to-globule transition where aqueous solutions shift from clear to opaque with increasing temperature. The thermoresponsive behavior of PNIPAM is favorable for sprayable smart window coatings for their ability to filter out light and heat from solar radiation. However, the presence of TMA, which allows PNIPAM coatings to bind to glass substrates, can lead to irrecoverable opacity due to crosslinking within the copolymer chain. Cloud point testing was utilized to characterize the optical response of PNIPAM-co-TMA over several thermal cycles as irrecoverable transmittances can be observed when the TMA crosslinks within the copolymer chain. However, systems composed of 95% mol of water and 5% mol of DMSO were able to recover their original clarity across various concentrations of TMA. These results are significant because co-nonsolvency allowed access to the collapsed, opaque, state using solvent mixtures instead of temperature. This may be advantageous for coating processes. Various co-nonsolvent systems were processed into coatings through either spin or drop coating. Finally, contact angles at 23°C and 60°C were collected for a coated slide. At room temperature, below the cloud point temperature, the coated slide had a contact angle of approximately 21°. When the coated slide was heated to 60°C a contact angle of 52° was measured. These results verify that the PNIPAM-co-TMA solution maintains the characteristic hydrophilic/hydrophobic phase change after the coating grafts onto the glass and subsequently permits this research to impact the use of polymer responsive coatings to improve energy efficiency.

Fabian Rodriguez

I joined PREM in Spring of 2022. I am currently pursuing a bachelors degree in Mechanical Engineering with a minor in Chemistry. I plan on pursuing a PhD in Material Science/Engineering, or Chemical Engineering. In Summer of 2022 I attended an REU at the University of Minnesota where I researched the role of solvent composition on the processing of PNIPAM copolymers for production of a stimuli responsive smart window coating. Since then, I have worked on two projects. The first centered around determining the ideal processing parameters to produce nutritionally dense Pullulan nanofibers. The second project I have been apart of has focused on using PNIPAM nanofibers to create a hydrogel biosensor.







March 30 – April 1, 2023 @Texas State University Campus

STUDENT POSTER PRESENTATIONS

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The Investigation of the Injectability and Cytocompatibility of Dynamic Poly(ethyleneglycol) Hydrogels

<u>Mackenzie U. Otakpor</u>¹, Andi Crowell², Kushal Thapa¹, Thomas FitzSimons², McKenzie Siller¹, Adrianne Rosales², Tania Betancourt¹ ¹Texas State University McKetta Department of Chemical Engineering, The University of Texas at Austin

Abstract:

Hydrogels are composed of hydrophilic polymers that are cross-linked to form a network. Hydrogels are often used to mimic the extracellular matrix (ECM), which contains macromolecules and minerals that aid in the physical and chemical support of cells. Hydrogels have found applications in biomedicine as tissue engineering scaffolds, wound healing materials, and drug delivery devices. Dynamic hydrogels, specifically, contain crosslinks that can be modulated by a range of internal and external stimuli, making them uniquely suitable to changing tissue microenvironments or to the need for on-demand drug release. A 4-arm poly(ethyleneglycol) macromer with benzal-cyanoacetamide end groups (PEG-RBCA) and 4arm poly(ethyleneglycol) macromer with thiol end groups (PEG-thiol) was used in this work to create dynamic hydrogels. The hydrogels were further loaded with poly(ethylenedioxythiophene) (PEDOT) nanoparticles which act as photothermal agents, enabling laser-induced modulation of hydrogel crosslinking by affecting the equilibrium of the dynamic bonds. The injectability and cytocompatibility of the hydrogels were investigated. To better understand the injectability and the mechanical compatibility of the hydrogels with the host tissue, we studied the rheological properties of the hydrogels as well as examined the injection force required for the administration of the hydrogels. To investigate the cytocompatibility of the hydrogels, two cell viability assays were used: Live/Dead assay and 3-(4,5dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium (MTS) assay. Studies were conducted with fibroblast cells and human MDA-MB-231 breast cancer cells. The goal of these studies was to examine the potential of these dynamic hydrogels for biomedical applications. The injectability studies demonstrated that the hydrogels are injectable with a clinically relevant force and the preliminary cell viability studies demonstrated that the hydrogels are cytocompatible.

Biography of Presenter:

Mackenzie Otakpor is an undergrad senior at Texas State University with a major in biology, a minor in biochemistry, and a pre-med concentration. At Texas State University she is an honors student as well as a researcher in the Department of Chemistry and Biochemistry working under Dr. Jennifer Irvin and Dr. Tania Betancourt. Her research at Texas State deals with conducting polymers for the rapid electrochemical detection of diseases specifically the MUC-1 gene as well as hydrogel cytocompatibility. After her undergrad, she plans on attending medical school.





Temperature-Dependent Self-Assembly Remodeling by a Polyether Perylene Diimide in Water

Adrian Fernandez¹, Mireya McKee², Pedro Rodriguez¹, and Sean M. Kerwin^{1,2,3} ¹Department of Chemistry & Biochemistry, Texas State University ²College of Pharmacy, University of Texas at Austin ³Materials Science, Engineering, and Commercialization Program, Texas State University

Abstract

We report a novel Perylene diimide (PDI) bearing polyether side chains that displays reversible, temperature depended remodeling of two spectroscopically distinct self-associated forms. We describe the synthesis of this PDI (TEL-045) and its self-association behavior in solution as determined by UV/Vis, fluorescence, and resonant light scattering spectral analysis. TEL-045 forms monomeric, emissive species in solution in organic solvents. In aqueous solution, TEL-045 undergoes self-association to produce a non-emissive state. As the temperature of aqueous solutions of TEL-045 are increased, the degree of self-association increases, and a new type of self-associated, emissive species is formed. We believe this is the first report of reversible, temperature-dependent switching between H- and J-type self-association of simple, non-chromophore-modified PDIs.



Biography of Presenter

Adrian Fernandez is currently a graduate student in the M.S. Biochemistry program at Texas State University and a graduate research assistant conducting research in the field of Materials Science as part of the Partnership for Research and Education in Materials (PREM) program. Adrian graduated from the University of Texas in Austin having received his B.S. biochemistry degree in 2020 followed by industry experience as an oenologist and as a laboratory associate at a clinical multiplexed immunoassay testing laboratory.





Photothermal Modulation of Drug Release from Dynamic Hydrogels

 <u>Kushal Thapa</u>,¹ Thomas FitzSimons,² Mckenzie Siller,³ Mackenzie Otakpor,³ Edgar Torres,³ Joanna Zepeda,⁴ Anne Crowell,² Lillian Roe,⁴ Adrianne Rosales,² Tania Betancourt¹,³
¹ Material Science, Engineering and Commercialization Program, Texas State University, San Marcos, TX
² McKetta Department of Chemical Engineering, The University of Texas, Austin, TX
³ Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX
⁴ Department of Biology, Texas State University, San Marcos, TX

Abstract

Hydrogels are a three-dimensional network of crosslinked hydrophilic polymers. Dynamic covalent bonds (DCBs) can be utilized as crosslinks to provide hydrogels with phase-reversible and stimuli-responsive properties. In our research, we selected one of such DCB, thia-conjugate bond, as crosslinks in our polyethylene glycol (PEG) based hydrogel. We investigated the thermal response of this hydrogel with the aim of developing an on-demand, pulsatile drug delivery system. Further, we incorporated poly(ethylenedioxythiophene) or PEDOT nanoparticles within the hydrogel to facilitate photothermal modulation of the drug release.

We synthesized the hydrogels using Michael addition of thiol-ene pairs from four-arm PEG thiol (PEG-SH) and four-arm PEG benzylcyanoacetamide (PEG-BCA). PEDOT nanoparticles, synthesized using an emulsion polymerization process, were entrapped within the hydrogel to act as photothermal agents. These nanoparticles, owing to their high absorbance in the near-infrared spectrum, show a rapid increase in temperature when irradiated with 808 nm laser. BSA-FITC, a fluorescently labeled protein, was loaded into the hydrogel-PEDOT complex and its release behavior into buffer upon direct thermal stimulation showed time-dependent release while upon photothermal stimulation with 808-nm laser showed a more controlled, time-independent release. The hydrogel-PEDOT complex was also shown to be injectable through a 28-guage hypodermic needle. The biocompatibility of the hydrogel-PEDOT complex was characterized on MDA-MB-231 cell line using the MTT assay and the results showed that this complex is not cytotoxic. Our dynamically crosslinked hydrogel loaded with PEDOT nanoparticles showed photothermally stimulated drug release in a clinically relevant environment.

Biography of Presenter

Kushal Thapa is a current doctoral student in the Materials Science, Engineering, and Commercialization program at Texas State University. He completed his B.S. in Biomedical Engineering and M.S. in Electrical Engineering. His experience, skill set and research interest spans material characterization, synthesis and testing of bioengineered systems, digital signal processing, machine learning and A.I., and programming. He also has start-up business experience. His company, based on smart electricity monitoring device, won first place in the 2022 TXST New Ventures competition. He has so far authored a few conference papers and one journal article in the field of digital communications. His current research with Dr. Tania Betancourt focuses on the design of dynamic thermo-responsive hydrogels for drug delivery application.





Dynamic, reversible cross-linked hyaluronic acid-based hydrogels for drug delivery

<u>Jessica Peterson</u>¹, Kushal Thapa², Tania Betancourt³ ^{1,2,3}Texas State University: Department of Chemistry and Biochemistry ^{2,3}Texas State University, Materials Science Engineering and Commercialization

Abstract

Hyaluronic acid (HA), is an abundant, viscous mucopolysaccharide in the human body. When chemically modified, HA can become an integral component of dynamic hydrogels. Hydrogels are three-dimensional, cross-linked networks of hydrophilic polymers. The unique properties of hydrogels and their tunability make them highly suitable for drug delivery and tissue engineering applications. These dynamic HA crosslinked hydrogels can be derived by functionalizing and chemically cross-linking reactive groups along the polysaccharide chain. In this work, HA is modified through three steps to generate HA-benzoacetoacetamide (HA-BCA), which can undergo reversible crosslinking with 4-arm-PEG thiol (PEG-SH) resulting in a hydrogel with dynamic properties. To prepare this, HA was modified into hyaluronate-azide (HA-Azide) through its carboxyl group with Azido-PEG3 -amine. HA-Azide was then modified via coppercatalyzed click chemistry to form HA-cyanoacetamide (HA-CA). A Knoevenagel condensation was then used to attach a benzaldehyde to HA-CA to make HA-BCA. Future work will show that hydrogels can be synthesized by mixing HA-BCA with PEG-SH. Conductive polymeric nanoparticles of poly(3,4-ethylenedioxythiophene) (PEDOT) will be added to the hydrogels to act as photothermal agents. The addition of these PEDOT nanoparticles will allow the extent of crosslinking of the hydrogels to be thermally controlled and offers the ability to tune the mechanical and transport properties of the system through laser stimulation. In preparation for next steps, 100-nm nanoparticles that absorb light in the near infrared range and that offer photothermal properties were prepared using an oxidative emulsion polymerization process. This research reports the functionalization, synthesis, and characterization of these dynamic HA based hydrogels.

Biography

Jessica Peterson is a 'second-degree seeking' undergraduate and biochemistry major at Texas State University. She completed her first Bachelor's in Anthropology also at Texas State. As part of the Department of Anthropology her research focused on the postmortem interval and decomposition processes for human remains at the Forensic Anthropology Research Facility. Currently, Jessica is a member of the Betancourt Research Group at Texas State University. The Betancourt lab focuses on perusing emerging research in cancer immunotherapies. Previously her research projects have focused on the synthesis/development of photothermal nanoparticles used to induce immunogenic cell death in breast cancer. The completion of this project lead to a



published peer-reviewed paper in the ACS Journal of Applied Polymer Materials. Her current research focuses primarily on the synthesis and characterization of hyaluronic acid cross-linked hydrogels to be used as drug-delivery systems in targeted cancer immunotherapies.



Optimization of Precursor Functionalization for the Synthesis of Dynamic Hydrogels

<u>McKenzie Siller</u>,¹ Kushal Thapa,² Thomas FitzSimons,³ Joanna Zepeda,⁴ Anne Crowell,³ Adrianne Rosales,³ Tania Betancourt^{1,2}

¹Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX ²Material Science, Engineering and Commercialization Program, Texas State University, San Marcos, TX ³McKetta Department of Chemical Engineering, The University of Texas, Austin, TX ⁴Department of Biology, Texas State University, San Marcos, TX

Abstract

Hydrogels are a three-dimensional network of crosslinked hydrophilic polymers. The tissue-like properties of hydrogels make them suitable as drug delivery systems, wound dressing materials, or scaffolds for soft tissue repair. The chemistry used for crosslinking the hydrophilic polymers that make up the hydrogel can be judiciously selected to provide the hydrogel with tunable properties. Depending on the crosslink identity, the resulting hydrogel can be made to respond to external or internal stimuli such as pH, mechanical stress, and heat by swelling, shrinking, dissolving or solidifying. In our research, we used Michael addition of thiol-ene functional pairs from four-arm PEG thiol (PEG-SH) and four-arm PEG benzylcyanoacetamide (PEG-BCA), respectively, to synthesize hydrogel via the formation of reversible covalent bonds. The nature of these reversible crosslinks is of exothermic nature, making the hydrogel thermosensitive and allowing it to shift between gel and sol states upon thermal stimuli. In this work, the syntheses of PEG cyanoacetamide (PEG-CA), the precursor to PEG-BCA, and of PEG-BCA are being optimized to yield a higher percent functionalization and thereby improve the crosslinking ability of the reversible hydrogel precursors. Specifically, the effect of reagent molar ration on the percent functionalization is being investigated with the aid of proton nuclear magnetic resonance (H-NMR) and absorption spectroscopy.

Biography of Presenter

McKenzie Siller is an undergraduate junior pursuing a Bachelor of Science in Biochemistry. Since

a freshman in high school, McKenzie continued her research journey into college and hopes to continue further with a masters or PhD in biomedical engineering. She is involved in PREM-CIMA, SACNAS, the Biochemistry Society, SPE and more.





Electroactive polymer-magnetic nanoparticle nanofiber composites for nerve regeneration

Nicholas Lontkowski¹, Adelyne C. Towne¹, Marvin D. Santiago¹, Nicolas Muzzio², Gabriela Romero-Uribe², and Jennifer A. Irvin¹

¹ Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX 78666 ² Department of Biomedical Engineering and Chemical Engineering, University of Texas at San Antonio

<u>Abstract</u>

Here we report the fabrication of a hybrid synthetic alternative for nerve tissue engineering. Electrospinning of biocompatible polycaprolactone is used to produce porous and highly ordered nanofibers that resemble the structure and organization of native spinal cord tissues providing a suitable environment to promote the adhesion and directional growth of nerves. These oriented nanofibers are coated with inherently conducting polypyrrole to provide an electrically conductive medium for external stimulus to enhance cellular growth and connectivity. Furthermore, the fibrous scaffold is engineered with magnetic nanoparticles to provide a remote-controlled option for the delivery of electrical inputs through the generation of Eddie currents when exposed to wireless alternating magnetic fields. The biocompatibility and neural tissue regeneration properties of these nanocomposites is investigated in detail.

Biographies of Presenters

Nicholas Lontkowski is pursuing a M.S. in Chemistry degree at Texas State University. He received his B.S. in Biochemistry from Texas State in 2022. Nicholas plans to pursue a Ph.D. with a focus on Environmental Sustainability so that he can create materials with reduced carbon footprints.

Adelyne Towne is a sophomore undergraduate biochemistry major at Texas State University. In summer 2021, she participated in Texas State University's Department of Energy-funded STEM Undergraduate Research Experience. Adelyne is planning to seek a Ph.D. in Biochemistry to prepare for a career in biomedical research.







Charge Transfer Through Individual DNA Molecules, Measured By Mechanically-Detected Electric Charge Sensing

<u>Rigo Mayorga-Luna</u>,¹ Noah Austin-Bingamon,¹ Binod D.C,¹ Damilola Runsewe,² Mitchell Ford, ¹ Tania Betancourt,² and Yoichi Miyahara, ¹

¹ Department of Physics, Texas State University, San Marcos, TX 78666² Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX 78666

Abstract

DNA has gained interest for use in novel nano-scale devices, particularly as a charge transfer medium for molecular nano-electronics. A thorough understanding of the electrical properties of charge transfer mechanics within DNA molecules is required for practical use of such devices. Previous experiments have shown conflicting results regarding the classification of DNA molecules as conductors, superconductors, semiconductors, or insulators. To address this, a standard non-invasive and repeatable method is required to characterize DNA molecules. In this research, we characterize individual hybridized DNA molecules attached to gold via thiol linkers using a non-contact mechanical method. DNA self-assembled monolayers are grown on silicon-gold substrates and hybridized with gold nanoparticle-functionalized complementary DNA. Charge transfer through the DNA is measured via atomic force microscopy non-contact mechanical charge sensing at cryogenic temperatures. This method avoids issues related to differing setups during each experiment, such as physical contact or misplacement of probes. Our research aims to provide a standard method for accurately characterizing DNA molecules and their electrical properties, which could have important implications for the development of molecular nano-electronics.

Biography of Presenter

Rigo Luna is a Physics Masters's Student at Texas State University and received his B.S. in Physics from Texas State in 2019. During his time there, he has helped create electrical potential simulations in COMSOL of biased AFM tips as well as assisting in the fabrication and characterization of a spin-based qubit architecture. Current research interests are characterization of Au nanoparticle energies by utilizing AFM methods. He is currently a Graduate Assistant under the oversight of Dr. Yoichi Miyahara lab whose work and research includes applications of advanced scanning probe microscopy techniques geared toward material nanometer scale characterization.





Chemical Modification of Polymer Nanofibers

Adelyne Towne¹, Madeleine Pastore¹, Marvin Santiago¹, Zachary Brotherton², Nathaniel Lynd², Jennifer Irvin¹ ¹ Department of Chemistry and Biochemistry, Texas State University ² McKetta Department of Chemical Engineering, University of Texas at Austin

Abstract

Polymer nanofibers, which possess high surface area and flexibility, can be prepared via a process known as electrospinning, in which a high voltage is applied to a concentrated polymer solution as it is extruded. The solvent evaporates, and the resultant polymer nanofibers are collected on a grounded plate or rotating drum. Inexpensive, commodity polymers can be used to prepare polymer nanofibers in this fashion, with the nanofiber properties dependent on the properties of the commodity polymer. The functional groups of the polymer can be modified after electrospinning to covalently bond reactive molecules that can be used to graft new polymers to the surface of the nanofibers. This poster will present attempts to covalently bond aromatic heterocycles to polymer nanofibers in order to graft electroactive thiophene-based polymers to the nanofibers. The resultant graft copolymers would potentially be useful for applications including biomedical materials, sensors, water purification, and energy storage.

Biographies of Presenters

Adelyne Towne is a sophomore undergraduate biochemistry major at Texas State University. In summer 2021, she participated in Texas State University's Department of Energy-funded STEM Undergraduate Research Experience. Adelyne is planning to seek a Ph.D. in Biochemistry to prepare for a career in biomedical research.



Madeleine Pastore is a junior undergraduate chemistry major at Texas State University. In summer 2022 she was a Texas State University CheMIE REU participant. She hopes to pursue a PhD so that she can lead materials chemistry and environmental engineering research.





Ruthenium-Chromium Oxide Aerogel Electrocatalysts: Structure, Oxygen Evolution Activity and Stability

<u>Jesus Adame Solorio</u>,¹ Kathleen Bailey,¹ Christopher P. Rhodes¹ ¹Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX 78666 *email: <u>cprhodes@txstate.edu</u>; website <u>http://rhodes.wp.txstate.edu/</u>

Abstract

Catalysts with enhanced activity and stability are needed for the anodic oxygen evolution reaction (OER) occurring in proton exchange membrane (PEM) water electrolyzers. Ruthenium-oxide based catalysts have shown the highest reported activities of any acidic OER catalysts, but their instability is a major roadblock for wider use. We investigated the effect of temperature treatment in air on Ru-Cr and Ru-oxide aerogel structure and electrochemical properties as an approach to increase the OER stability and activity. The thermally treated Ru-Cr oxides showed increased surface area and porosity relative to Ru-oxides. Electrochemical testing revealed that Cr incorporation improved catalytic OER activity. Higher temperature treatments also resulted in higher OER catalytic activity for Ru-Cr oxides whereas Ru-oxides showed higher OER catalytic stability relative to a commercial RuO2. The ruthenium-chromium catalyst treated at 500°C showed more than 16 times higher mass activity and similar stability compared to a commercial RuO_2 ; its activity remained higher than the commercial RuO_2 after applying a constant potential of 1.6 V during 13.5 h (accelerated durability test). The ruthenium oxide catalyst treated at 600°C exhibited higher stability than the commercial RuO₂ after the accelerated durability test. Further work to explore different temperature ranges and Ru-Cr compositions can provide OER electrocatalysts with high activity, improved stability and lower cost.

Biography of Presenter

Dr. Jesus Adame Solorio has been involved in renewable energy research for the last ten years. Since his undergraduate studies in Mexico, his primary interest has been the development of nanostructures for different applications in green chemistry such as the development of nickel

nanocatalysts for the hydrogen evolution reaction and the study of the plasmonic effect of gold nanoparticles in organic solar cells. During his studies in the Materials Science, Engineering, and Commercialization (MSEC) Ph. D. program at Texas State University he obtained second place in the 60 second Elevator Pitch competition during the 2018 Entrepreneur Intensive Course and was awarded the 2018 Wilson Latin American Scholarship. Also, he has recently graduated from the Ph. D. in Materials Science, Engineering and Commercialization program at Texas State University in December 2022.





G-triplex based Biosensor for the Detection of Calcium(II) ions

<u>Elizabeth Williams</u>,¹ Mitchell Myhre,¹ Christina Kuczynski,¹ Samantha Unuigbokhai,¹ Sean M. Kerwin^{1,2} ¹Department of Chemistry & Biochemistry, Texas State University ²Materials Science, Engineering, and Commercialization Program, Texas State University

Abstract

G-quadruplex DNA structures, which are formed from planar stacks of G-tetrads, have recently received attention as recognition elements in bioanalytical assays. DNAzymes are functionally active, synthetic single-stranded DNA molecules that are capable of catalyzing biological reactions similarly to proteins or RNAzymes. One class of DNAzymes mimic peroxidase and catalyze the oxidation of luminol or ABTS in the presence of H_2O_2 . These peroxidase-mimicking DNAzymes consist of G-quadruplex structures, which provide a suitable hydrophobic hemin binding pocket that contributes to oxidation enhancement. G-triplex DNA structures, which are characterized by G:G:G triads stabilized by Hoogsteen hydrogen bonding, were originally identified as folding intermediates for G-guadruplexes. More recently, certain truncated Gguadruplex forming sequences have been shown to form stable G-triplex structures; although, the "rules" for which sequences fold into stable G-triplexes are not well defined. While Gguadruplex-based peroxidase mimicking DNAzymes have been employed in a number of sensor designs, there have been no examples of chemiluminescence-based DNAzymes based on Gtriplex motifs. We hypothesized that the G-triplex could function as a type of peroxidase mimicking DNAzyme that could have some advantages in sensor design. Here we show that a variety of previously-described and newly reported G-triplexes are able to catalyze the oxidation of luminol to produce chemiluminescence. Furthermore, various G-triplex forming sequences can be used to design label-free G-triplex based biosensors for the detection of Ca²⁺ ions. A simple and costeffective assay such as this would be beneficial to the diagnostic field for the current techniques of Ca^{2+} ion detection requires sophisticated instrumentation and complicated sample preparation.

Biography of Presenter

Elizabeth Williams was raised in north Houston, Texas, and went to the Woodlands Highschool. In 2016, she moved to San Marcos to attend Texas State University studying Biochemistry with a minor in Biology. In 2020, she began her graduate degree studying Biochemistry and has expanded her learning by teaching undergraduate biochemistry students as an instructional assistant. In April of 2022, she was awarded an outstanding graduate instructional assistant award from the department of Chemistry and Biochemistry at Texas State University. Elizabeth began working under Dr. Sean Kerwin as an undergraduate junior studying the changes in functionality of G-triplex and G-quadruplex structure when contained in different salt concentrations.





Poly(lactic-co-glycolic acid)/Polyethylenimine nanocarriers of microRNA for reprogramming neuroblastoma cancer cells.

Josue Osorio, Tania Betancourt, Du Liqin ¹ Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX 78666

Abstract

Neuroblastoma is a type of childhood cancer diagnosed within the first years of life but begins metastasis during fetal development. This cancer develops in the nerve tissue, and spread in the adrenal glands, spinal cord, or neck, creating immature nerve tissue or neuroblasts. Proteincoding and nonprotein-coding genes responsible for neuroblastoma cell differentiation have been discovered, and studies have shown that microRNAs (miRNAs) help to induce neuroblastoma cell differentiation and have oncosuppressive functions depending on the cell line. MicroRNAs are small molecules that bind to proteins to activate/deactivate or regulate gene expression by binding to the messenger RNA (mRNA), thus preventing protein translation.MicroRNAs are ideal as opposed to viral vectors because of their minimal immunogenic response, and their high reliability since most miRNAs can be chemically synthesized due to their short nucleotide sequence. Because of the negative phosphate groups in the miRNAs, and the presence of endo- and exonucleases within the cell, it is important to find a reliable nano vector. This experiment aims to develop a PEI-miRNA polyplex. encapsulated in PGLA nanoparticles to be delivered to neuroblastoma cancer cells for differentiation to healthy nerve cells. The microRNA used was chemically synthesized, the polyplex was prepared using nitrogen over phosphate ratio of RNA (N:P) to neutralize the negative charges of the miRNA with the positively charged PEI, and the complex formation was confirmed with gel electrophoresis. The results show that at a neutral charge, the RNA migrates slower. The polyplex was then encapsulated in PLGA nanospheres.

Mr. Osorio is an undergraduate student at Texas State University. He has completed 2 months of STEM undergraduate research using CRISPR-Cas9 and other molecular biology techniques, and participated in an REU at UT Austin where he worked on understanding the molecular orientation of an organic layer placed on top of a silicon solar cell for improved solar energy generation. His personal interests are in sport motorcycles, science communication, finance, personal development, and entrepreneurship, and his educational interests are in food production, synthetic biology, and the natural materials of plants and insects.





Effect of Oxygen Evolution Catalyst Layer Composition on Proton-Exchange Membrane Water Electrolyzer Performance and Durability

<u>Michael E. Urena,</u>¹ Jose Fernando Godinez-Salomon,¹ and Christopher P. Rhodes^{1,2} ¹Department of Chemistry and Biochemistry, Texas State University, San Marcos, TX, 78666, USA ²Materials Science, Engineering, and Commercialization Program, Texas State University *email: <u>cprhodes@txstate.edu</u>; website <u>http://rhodes.wp.txstate.edu/</u>

Abstract

Proton-exchange membrane (PEM) electrolysis is a promising technology to produce clean hydrogen at large scale and aids efforts to increase use of renewable energy sources. Currently, iridium oxide-based oxygen evolution reaction (OER) catalysts are used for commercial PEM electrolyzers. Ruthenium oxide (RuO₂) is more active for OER and less expensive than iridium oxide, but RuO₂ catalysts lack stability under the acidic environment present during operation. To improve the stability of RuO₂ OER catalysts, we are investigating the performance and durability of RuO₂ and ruthenium-titanium oxide catalysts in electrolyzer membrane electrode assemblies (MEAs). The performance and durability of MEAs with commercial catalysts (iridium oxide and ruthenium oxide) are evaluated to establish a performance baseline and an endurance testing protocol suitable to evaluate novel Ru-based catalysts. Ink formulation and spray parameters were established to deposit the OER catalyst layer directly onto the membrane and obtain a uniform catalyst layer with controlled catalyst loading. Commercial ruthenium oxide MEAs exhibited rapid degradation (~30 min) under the testing protocol used providing a basis for evaluation of a metal-substituted ruthenium oxide catalyst under similar conditions. The degradation time of RuO₂ MEAs was found to depend on the current density and voltage. Tisubstituted ruthenium oxide was synthesized hydrothermally with a nominal titanium concentration of 20 at. % and thermally treated in air at 450 °C. X-ray diffraction showed peak shifts consistent with the incorporation of Ti into the rutile RuO₂ structure.

Biography

Michael Urena is a graduate research assistant in the Dept of Chemistry and Biochemistry at Texas State University. He received his BS in Chemistry & Applied Mathematics from Texas State University in Spring 2021, where he then continued in the MS Chemistry program expanding on his undergraduate research in the Rhodes group as a PREM CIMA researcher. Some of his most distinguished accomplishments include receiving an Undergraduate Research Fellowship from the Honors College in 2020 and a Certificate of Excellence from the Dept. of Chemistry and Biochemistry for outstanding performance in General Chemistry I, II courses the 2016-2017 academic year.





Photothermally Responsive Dynamic Hydrogels Incorporating Reversible Thiol/Ene and Irreversible Maleimide/Thiol Crosslinking for Pulsatile Drug Delivery

<u>Edgar Torres</u>,¹ Kushal Thapa,² Thomas FitzSimons,³ Mckenzie Siller,¹ Joanna Zepeda,¹ Adrianne M. Rosales,³ Tania Betancourt^{1,2}

¹Department of Chemistry and Biochemistry, Texas State University ²Materials Science, Engineering and Commercialization Program, Texas State University ³McKetta Department of Chemical Engineering, The University of Texas at Austin

Abstract

Hydrogels are three-dimensional hydrophilic polymer networks with tissue-like properties that have been used in biomedical applications for several decades. In our laboratory, a pulsatile drug delivery system based on dynamic poly(ethyleneglycol) (PEG) hydrogels crosslinked via thiol/ene Michael addition was previously explored. These hydrogels were designed to be photothermally activated upon irradiation of embedded poly(ethylenedioxythiophene) (PEDOT) nanoparticles. While showing great promise, the dynamic nature of the crosslinks of these hydrogels led to the uncontrolled hydrogel dissolution and consequent release of entrapped agents when no stimulation was applied when in an unconstrained aqueous environment. In this work, 4-arm-PEG-Maleimide (PEG-Mal) is investigated as a potential solution providing a secondary crosslink to contain the unwanted release. To synthesize the hydrogel, a Michael addition of thiol-ene functional four-arm PEG-benzylcyanoacetamide, PEG-thiol, and PEG-Mal was conducted. Various molar ratios of the three precursors were explored. The hydrogel was loaded with PEDOT nanoparticles to provide it with photothermal properties, and BSA-FITC, a fluorescently labeled protein, acted as a therapeutic mimic. The release of BSA-FITC upon application of heat or laser irradiation of the hydrogels was confirmed visually and spectroscopically. Results showed that no undesired release of BSA-FITC occurred from hydrogels that included PEG-Mal, in contrast to those lacking these stable crosslinks. Further studies will be carried out to verify the addition of PEG-Mal as a viable option for the preparation of hydrogels for the pulsatile release of therapeutic agents.

Biography of Presenter

Edgar Torres, a student at Texas State University, will receive a Bachelor of Science in Chemistry, a Bachelor of Fine Arts in Communication Studies, and a minor in Biology when he graduates in May 2023. He is currently working on developing photothermally responsive hydrogels for drug delivery applications in the Betancourt Research Group. Prior to this, he conducted two internships at Eli Lilly and Company, where he worked on methods for both synthesizing non-coded amino acids for peptide synthesis and identifying proteins of interest for potential therapeutics. Furthermore, he is a current Undergraduate Research Training Initiative for Student Development (U-RISE) Scholar and a Houston-Louis Stokes Alliance for Minority Participation (H-LSAMP) Scholar.





Laser Synthesis of Metastable Materials for Enhanced Catalysis

<u>Warren Burke</u>,¹ Austin Gillette,¹ Edgar Torres,¹ Maddie Tello,¹ Jacob Armitage,¹ Edward Yu,² Ben Martin¹ ¹Department of Chemistry and Biochemistry, Texas State University, ²Department of Electrical and Computer Engineering, University of Texas at Austin

Abstract

Traditional solid state synthesis techniques typically generate highly crystalline, thermodynamically stable phases. However, low energy crystal faces have relatively low catalytic activities and phase segregation often prevents the formation of solid solutions. We hypothesize that rapid heating and cooling using a translating focused laser beam can overcome thermodynamic barriers by: limiting the extent of diffusion, exposing unusual crystal faces, and forming a high number of active defect sites. Here we explore the synthesis of two catalyst solid solutions from amorphous and crystalline precursors: $(Ti/Ta)O_2$, an anodic electrocatalyst, and $(Mo/W)S_2$, a hydrogen evolution catalyst. We find that the structures and compositions of our laser-synthesized products differ from those synthesized using conventional heating methods.

Biography of Presenter

Warren Burke is an undergraduate PREM researcher at Texas State University working on inorganic sol gel synthesis at Texas State University. Previous experience included working as a laboratory instructor assistant and online chemistry tutor. He is a student member of the ACS and a current member of the NSLS.





Metal-Substituted Ruthenium Oxides: Surface Electronic Structure, Oxygen Evolution Activity and Stability

<u>Kathleen O. Bailey,</u>¹ Luis A. Albiter,² Fernando Godinez Salomon,¹ and Christopher P. Rhodes^{1,2*} ¹Department of Chemistry and Biochemistry ²Materials Science, Engineering, and Commercialization Program, Texas State University, San Marcos,

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Abstract

Proton exchange membrane water electrolyzers (PEMWE's) allow electrochemical splitting of water into hydrogen and oxygen and can be powered by renewable energy sources (e.g. solar, wind), resulting in generation of "green hydrogen". The large-scale adoption of PEMWE's is hindered by the sluggish kinetics and cost of the oxygen evolution reaction (OER) catalyst at the anode. The current state-of-the-art OER catalysts are iridium-based; however, iridium is a rare element in the Earth's crust and is extremely expensive, resulting in high catalyst costs. Ruthenium oxide (RuO₂) OER catalysts are of interest due to their higher activity and lower cost compared to iridium oxide; however, RuO₂ is unstable and corrodes over time. By incorporating tantalum, niobium, or zirconium into ruthenium oxide at various concentrations, $Ru_{1-x}M_xO_2$ (M= Ta, Nb, Zr, x=0-50 at. %), the catalyst cost and stability can be potentially improved. X-ray photoelectron spectroscopy (XPS) was used to characterize the surface electronic structure of the $Ru_{1-x}M_xO_2$ catalysts. Preliminary XPS analysis shows that tantalum is at a +5-oxidation state, niobium is at a +5-oxidation state, and zirconium is at a +4-oxidation state. X-ray diffraction and scanning electron microscopy (SEM) characterization show that the addition of the metal substituents, Ta, Nb, or Zr, affected the overall structure and morphology of the catalysts. Preliminary rotating disk electrode results show that the addition of the metal substituents into ruthenium oxide have a significant effect on the OER activity of the synthesized Ru_{1-x}M_xO₂ catalysts. Our findings help to further the development of high activity, lower cost, and high stability ruthenium based OER catalysts that can improve the efficiency and lower the operating costs of PEMWEs.

Biography of Presenter

Kathleen Bailey is a senior undergraduate at Texas State University and has been a part of the Rhodes research group since June of 2021. Her undergraduate research focuses on surface characterization of ruthenium-based oxygen evolution reaction catalysts.





Mechanochemical Synthesis and Characterization of Ruthenium-Titanium Oxide Oxygen Evolution Electrocatalysts for Water Splitting

<u>Camden Caffey</u>, Fernando Godinez-Salomon, and Christopher Rhodes* Department of Chemistry and Biochemistry Texas State University, San Marcos, TX 78666 *email: cprhodes@txstate.edu; website http://rhodes.wp.txstate.edu/

Abstract

Proton-exchange membrane water electrolysis (PEM-WE) is a promising technology for sustainable, large-scale hydrogen production. However, the very harsh conditions found on the anode during the oxygen evolution reaction (OER), limit the choice of catalysts to platinum group metals (PGMs). Iridium-based materials have shown the best compromise of activity and stability under PEM-WE conditions, however, for large-scale systems (MW's or GW's), iridium scarcity in combination with high-catalyst loading (0.5-4.0 mg_{PGM}/cm²) becomes a serious technical and economic problem that limits wide-scale adoption of PEM-WEs. Ruthenium is a more abundant, cheaper, and more catalytically active than iridium, but its application has been limited due to significantly lower stability compared to iridium. Recently, our group has been working on the development and understanding of structures based on solution-phase synthesized RuTiO_x materials, which have shown improved stability [1]. Mechanochemical synthesis has demonstrated great value in the fabrication of heterogeneous catalysts at larger scales and with well-integrated structures. In this study, we evaluated a mechanochemical synthesis route to produce RuTiO_x materials. RuO₂ and TiO₂ were combined in a 50:50 ratio into a ball mill jar and was ball milled for 1, 5, 10, and 15 hours. The structure of RuTiO₂ was monitored using X-Ray Powder Diffraction. The increase of the ball-milling time reduced the size of particles, which would suppose more efficient catalysts in terms of the number of active sites, and increased the RuO₂:TiO₂ integration marked by the conversion of the TiO₂-anatase phase into a single rutile RuTiO₂ after 10 hours.

References

 Godínez-Salomón, J. F.; Ospina-Acevedo, F.; Albiter, L.; Bailey, K.O.; Naymik, Z.G.; Mendoza-Cruz, R.; Balbuena, P.B.; Rhodes, C.P. ACS Applied Nano Materials, 5 (8), 11752– 11775. <u>https://doi.org/10.1021/acsanm.2c02760</u>

Biography of Presenter

Camden Caffey is an undergraduate student at Texas State University and will receive a Bachelor of Science in Chemistry with a Pre-Medical concentration and a minor in Biology when she graduates in May 2023. She hopes to continue her education by going to medical school after she graduates.





Synthesis and Characterization of Nickel Hydroxide Cathodes for Rechargeable Alkaline Nickel-Zinc Batteries

Jaret A. Manley,¹ Cory M. Silguero,¹ Samuel W. Kimmel,² and Christopher P. Rhodes^{1,2*} ^{1,} Department of Chemistry and Biochemistry, Texas State University ²Material Science, Engineering, and Commercialization Program, Texas State University *email: cprhodes@txstate.edu; website http://rhodes.wp.txstate.edu/

Abstract

With an increase in concerns about the highly flammable electrolyte used in Lithium-Ion batteries, widely used in today's market, there exists a need for a new and safer battery for electrochemical energy storage. Alkaline batteries with a nickel cathode and zinc anode offer a safer alternative to lithium batteries. Al-substituted α -Ni(OH)₂ can potentially store more than one electron per Ni atom, increasing the energy density of the overall nickel-zinc cell. We investigate the effects of microwave reaction temperature and reaction duration on the electronic structure and local coordination environment of α -Al-Ni(OH)₂ nanosheets deposited onto carbon nanofiber paper (AI-Ni(OH)2@CNP) by Raman and X-ray photoelectron spectroscopy (XPS). XPS was used to probe the binding energy of N1s, O1s, Ni 2p core electrons and showed the reaction temperature alters the surface electronic structure Raman spectroscopy was used to probe the Ni-O lattice, hydroxyl modes of α -Ni(OH)₂ and modes of other residual synthetic precursors incorporated into the structure. Raman was collected using a Horiba Labram HR Evolution confocal Raman Spectrometer using backscattering geometry and a 600 groves per nm grating at a 10% ND filter on a 514 nm Argon-ion laser. Varying the microwave reaction temperature and reaction duration results in differences in surface agglomeration, XPS binding energies, and Raman vibrational mode frequencies of the Al-Ni(OH)2@CNP. Understanding and correlating changes in microwave reaction conditions with changes in the electronic structure and local coordination environment of Al-Ni(OH)2@CNP can further the development of safer nickel-zinc batteries.

Jaret Manley (left): I am currently a Senior at Texas State pursuing a bachelor's in chemistry with



plans to continue here and achieve a master's in chemistry. I work under Dr. Christopher P. Rhodes in the synthesis of nanomaterials used for electrochemical storage, specializing

in the collection and analysis of Raman Spectroscopy.

Cory M. Silguero (right): Currently a senior chemistry major at Texas State who will be attending graduate school at the University of Texas in hopes to receive his PhD in chemistry. I conduct x-ray photoelectron spectroscopy (XPS) to analyze the chemical



and oxidative makeup of nanomaterials.


Improving Mixed Metal Oxide Electrocatalysts for Proton Exchange Membrane Water Electrolysis by Thermal Treatment Tailoring

Zachary G. Naymik,¹ Jose Fernando Godinez-Salomon,¹ Luis A. Albiter,² Christopher P. Rhodes,^{*1,2} ¹Department of Chemistry and Biochemistry ²Materials Science, Engineering, and Commercialization Program *email: cprhodes@txstate.edu; website http://rhodes.wp.txstate.edu/

Abstract

The increased demand for green renewable energy has made hydrogen a viable option for energy storage. Hydrogen produced by proton exchange membrane water electrolyzers produces storable hydrogen with only water and electricity and can provide a chemical feedstock that will lower total carbon emissions within multiple manufacturing sectors. Electrocatalysts for the anodic oxygen evolution reaction (OER) have sluggish kinetics, stability challenges, and currently require expensive and rare Ir-based catalysts. Ruthenium oxide (RuO₂) provides a higher OER activity and lower cost compared to iridium oxide; however, RuO₂ is less stable than IrO2. We recently reported that substitution of titanium into RuO₂ provides OER catalysts with improved stability. In addition to the effects of Ti, the thermal processing conditions impact structure and performance. In this study, the effects of thermal treatment temperature and atmosphere on the structure, OER activity, and stability of ruthenium-titanium oxide electrocatalysts were determined. Ruthenium-titanium oxides using an 80:20 atomic ratio of Ru:Ti (notated as Ru_{0.80}Ti_{0.20}O₂) were prepared using a hydrothermal synthesis route, thermally treated at various temperatures and atmospheres, and characterized by x-ray diffraction, nitrogen physisorption, and rotating disk electrode measurements. Lowering the treatment temperature increased the catalyst's Brunauer-Emmett-Teller surface area. Treatment in oxygen atmosphere significantly increased the initial OER mass activity compared to Ru_{0.80}Ti_{0.20}O₂ treated in air at the same temperature. Accelerated durability tests showed that the mass activity retained of the catalyst was improved using a lower thermal treatment temperature. The results of this study further the understanding of OER catalyst design and provide a path developing OER catalysts with improved activity and stability, and lower cost that contribute to the goal of realizing a widespread hydrogen-based economy. The next steps in this study include characterizing differences in the surface of each catalyst with x-ray photoelectron spectroscopy and determining rate of dissolution of catalyst during OER by Inductively coupled plasma mass spectroscopy.

Biography of Presenter

Zachary Naymik is a M.S. chemistry student at Texas State University. He earned his B.S. in chemistry at Texas State University. Zachary works as a graduate research assistant studying advanced energy materials in Dr. Christopher Rhodes' lab. Zachary has given a presentation to the Texas State University Chemistry and Biochemistry department and plans to present a poster at the ACS spring 2023 conference. He has been an author on one publication and has a second manuscript in progress.





Tensiometric Characterization of Photosurfactants

<u>Viola Fieglein</u>, Makena Burns, Emily Cwiklik, Scott Barrett and William Brittain Department of Chemistry and Biochemistry, Texas State University

Abstract

Surfactant molecules, found mainly in soaps and cleaning products, can be used for drug delivery via reversible micellization. Through exposure to light, azobenzene photosurfactants demonstrate a capacity for forming reversible micelles. Micelle formation occurs more readily with the *trans*-isomer rather than the *cis*-isomer. The aim of this study is examining how different functional groups on azobenzene interact with UV-light and impact critical micelle concentration (CMC) value using both nuclear magnetic resonance spectroscopy methods as well as contact angle measurements revealing changes in interfacial tension. CMC value is the detectable region where aggregation begins. The research looked into two types: anionic and cationic photosurfactants; each compound's CMC values were calculated. As per the data, micelles are not formed as easily



for anionic photosurfactants in *cis*isomer compared to *trans*-isomer since their CMC value is higher. This may be due in part to the inhibition of tight packing in the *cis*isomer. Moreover, it was observed that the compound with a trimethylammonium group had a larger CMC value compared to its counterpart with imidazole.

Biography of Presenter

Viola Fieglein is a Chemistry major with a minor in Biology at Texas State University, expected to graduate in May 2023. In addition to her academic pursuits, Viola has gained valuable experience

as an instructional assistant for organic chemistry and quantitative analysis, where she ensures safety procedures are followed and answers chemistry-related questions for lab attendees. She also works as an undergraduate research advisor, analyzing kinetics via UV-Vis and NMR under the advisement of Dr. Brittain. Viola has been an active member of the American Chemical Society Texas State Student Chapter, where she tutors her peers in chemistry. While she has not yet received any awards or honors for her work, she is dedicated to continuing her professional growth and achieving recognition for her contributions to the field.





The Synthesis, Separation and Characterization of Azobenzene Isomers

<u>Jacob Guerrero</u>, Scott Barrett, Makena Burns and William J. Brittain Department of Chemistry and Biochemistry Texas State University, San Marcos, TX 78666

Azobenzene is a ubiquitous organic chromophore that undergoes reversible *cis-trans* isomerization. Typically, UV irradiation leads to formation of metastable *cis*-isomer which reverts to the *trans*-isomer by either spontaneous thermal isomerization or visible light photoisomerization. As a chromophore, azobenzene advantages include photostability and facile synthesis of derivatives. By judicious aromatic substitution, properties like *cis*-isomer lifetime, molecular geometry, aqueous solubility, excitation wavelength, and melting point can be controlled. Azobenzene synthesis and characterization is a cornerstone of our research group. Published studies have included photopharmacology, reversible micellization of single strand DNA hybrids, *cis-trans* mechanoisomerization in elastomers, and the rate of phenyl rotation in the cis-isomer. Recently we have initiated research into reversible photoadhesives and solar



thermal fuels. A key to understanding isomeric differences in properties is the preparation and isolation of the *cis*- and *trans*-isomers. The isomers display distinct differences in UV-Vis spectra, NMR spectra and physical properties.

Biography of Presenter

Jacob Guerrero is an undergraduate student at Texas State University. He is a senior majoring in Biochemistry with a minor in Exercise and Sport Science. He is currently doing research in a synthetic organic chemistry. He has a fascination with synthesizing new organic compounds that have applications in renewable energy.





Polarization Dependent Raman of GeCSn for Defect Identification

Layne Sauer¹, Augustus W. Arbogast¹, Tuhin Dey², Mark Holtz^{1,2}, Mark A. Wistey^{1,2} ¹Department of Physics, Texas State University, San Marcos, TX 78666 ²Materials Science, Engineering, and Commercialization Program, Texas State University, San Marcos, TX 78666

Abstract

Adding lasers and other active devices in silicon photonics would greatly increase the speed of data transfer between chips, which is especially important as multicore CPUs and GPUs increasingly fight over the narrow data paths to memory. However, common laser materials such as GaAs are incompatible with silicon. On the other hand, dilute germanium carbides such as Ge:C and GeSn:C emit light and can be grown directly within silicon CMOS electronic chips. Our group has previously been able to use Raman spectroscopy to roughly measure the concentrations of carbon and Tin in samples of germanium. These measurements roughly correlated to other techniques like XPS and RBS. With this study, we are studying the possibility of using Raman spectroscopy to measure and quantify defects in these same materials. Raman shift relies on the characteristics of bonds between the atoms. The bonds created by defects vary in direction and length compared to substitutional atoms, especially at carbon-carbon split interstitial sites, where two C atoms share a single Ge site. Polarization dependent Raman spectroscopy should allow us to isolate and view bonds that are only aligned in certain orientations in the crystal by using a halfwave plate and polarization analyzer. With defect bonds, we expect the forbidden and allowed modes of polarized Raman to reduce in difference as the defect bonds are less orientation dependent. My preliminary measurements show a distinct difference in the intensity of the Raman peak according to polarization, and the intensity is the same as samples of pure Ge. Polarization dependent Raman of more samples of the highly mismatched GeCSn alloy will further help distinguish between the effects of defects and "expected" behavior of the material. Future work will study samples with known defects for comparison, and also study the pressure dependence of both Raman and photoluminescence spectra to further separate the effects of defects from the overall band structure.

Biography of Layne Sauer

Layne is a Physics major at Texas State University working as an undergraduate researcher in Dr. Wistey's group studying highly mismatched alloys. Layne is also an active member of the Society of Physics Students and a learning assistant for the physics department.





Nanomaterials and van der Waals Heterojunctions for Electronic and Energy Applications

<u>Vinod K. Sangwan</u>,¹ J. Tyler Gish,¹ Anthony Martinez,² Abhishek Rawat,² Laura M. Clark,² Vineet K. Jayakrishnan,² Hannah Umoeka,² John Cavin,¹ Riddhi Ananth,¹ Emily A.Weiss,¹ James M. Rondinelli,¹ Efstathios I. Meletis,² Rajeshwar Krishnan,² Seong Jin Koh,² and Mark C. Hersam¹ ¹ Northwestern University, Evanston, Illinois 60208 ² The University of Texas at Arlington, Arlington, Texas 76019

Abstract

Van der Waals heterojunctions have emerged as promising materials systems to realize novel electronic, optoelectronic, and neuromorphic hardware circuits. Controlled synthesis, assembly, and fundamental characterization of passivated materials are becoming increasingly crucial for this class of materials due to extreme sensitivity to environmental effects. Thus, the purpose of this poster is twofold. First, I wish to present a snapshot of nanomaterials research and facilities from our group (Hersam) at Northwestern University and general user facilities on the campus. Research topics on nanomaterials, assembly, and characterization are chosen to spark ideas for future collaborations within the PREM partnership between NU MRSEC, the University of Texas at Arlington, and campuses. Second, I will discuss the initial results from existing PREM collaborations to complement more exhaustive presentations by PREM students. For example, I will showcase initial results on heterojunction devices where bulk Si semiconductor and two-dimensional SnO₂ quantum wells are separated by a thin tunnel barrier. In particular, memristive switching in SnO₂ quantum wells has been exploited to obtain relaxation oscillators operating in the MHz range. I will also present initial results in using ternary oxide materials for photoelectrochemical cells and discuss emerging optoelectronic applications.

Biography of Presenter

Dr. Vinod K. Sangwan is a Research Assistant Professor in the Materials Science and Engineering Department at Northwestern University (NU). He obtained a B.Tech. in Engineering Physics from the Indian Institute of Technology (IIT) Mumbai and a Ph.D. in physics from the University of Maryland (UMD) College Park. His research interests include nanomaterials, nanoelectronics, neuromorphic computing, renewable energy, and quantum information science. He has published over 100 peer-reviewed journal papers that have been cited more than 12,000 times. He recently received the 2021 IEEE



Chicago Outstanding Senior Research and Development award. Dr. Sangwan has mentored more than 30 graduate and undergraduate students and regularly participates in outreach activities and leadership roles in APS, MRS, and IEEE.



Fast Plasmonic Detection of Covid-19 Oligonucleotides on Solid Substrates

Vineet Kumar Jayakrishnan,¹ <u>Hannah Umoeka</u>,¹ Luis Dibert,¹ Anthony Martinez,¹ Chinmay Nitin Afzulpurkar,¹ Mileend Pankajbhai Sharma,¹ Vinod Kumar Sangwan,² Mark C. Hersam,² Seong Jin Koh¹ ¹The University of Texas at Arlington, Arlington, Texas 76019 ²Northwestern University, Evanston, Illinois 60208

Abstract

An ability to detect specific sequences of DNA or RNA of various pathogens, such as Covid-19, is critical for public health and national security. Although polymerase chain reaction (PCR) or reverse transcription PCR (RT-PCR) has been the gold standard for pathogen detection, it requires a substantial amount of time (>1 hour), trained personnel, and lab space. Here we present an approach that enables a fast, portable, and inexpensive detection of specific sequences of oligonucleotides. Using 67-mer oligonucleotides (oligos) having a Covid-19 sequence as a model system, we demonstrate that the Covid-19 oligos can be detected in less than 5 minutes on a solid substrate (silicon or glass) smaller than a thumb, with a dimension of 6 mm by 9 mm. In our approach, the Covid-19 oligos are sandwiched between a capture Au nanoparticle (C-AuNP) and probe Au nanoparticles (P-AuNPs), to form core-satellite nanoparticle conjugates, which are detected by the red shift of the plasmon resonance peak in UV-VIS spectroscopy. The total hybridization time to form the core-satellite conjugates is only 3 minutes, with a detection sensitivity currently as low as 50 pM. In addition, the absorbance change of the red-shifted plasmon resonance peak correlates with Covid-19 oligo concentrations, enabling a quantitative detection over a concentration range of at least 4 orders of magnitudes. The fabrication cost of the detection unit is currently less than 5 dollars, while much lower cost is expected as the detection units can be mass-produced using current semiconductor fabrication technology. Our approach has a potential to be used as a fast, portable, and inexpensive initial screening of various pathogens in the field. This work was supported by the National Science Foundation (DMR-2122128, ECCS-2031770, and DMR-1720139).

Biography of Presenter

Hannah Umoeka is a senior at the University of Texas at Arlington studying for her bachelor's in biomedical engineering with a minor in materials science and engineering. She was introduced to materials science in November of 2021 when she had the opportunity to join the Koh Lab and learn the ins and outs of research. Inspired by this experience, Hannah plans continue to graduate school to pursue research in materials science and bioengineering.





Design and Development of Aligned Ni₅P₄-Ni₂P/NiS Heterostructures for Enhanced Hydrogen Evolution Reaction (HER) Catalytic Activity

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²Environmental Science and Engineering, University of Texas at El Paso,

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³Department of Mechanical Engineering University of Texas at El Paso,

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Abstract:

The projection of developing durable and economic electrocatalysts for energy conversion is getting hot. Though demand for environmental-friendly energy sources is at its maximum, Ptgroup metals (PGM) are scarce and expensive, and the full potential of earth-abundant metals for substituting with PGM has yet to be exploited due to insufficient design strategies. The current study aims to optimize the electronic properties and modify the catalyst structure by enhancing the intrinsic catalytic activity and expanding the electrochemical active surface area. We report on synthesizing a 3D heterostructure of aligned Ni₅P₄-Ni₂P/NiS (plate/nanosheets) using a phospho-sulfidation process. An ultrathin nickel mesh is selected to facilitate the uniform transport of chemical vapors over the entire surface and provide spatial freedom for removing the produced hydrogen. The heteroepitaxial growth between Ni₅P₄-Ni₂P plates and NiS nanosheets inspires us to adopt the design of prickly pear cactus, entirely pertinent to the Southwest and Desert regions of the planet. The synergistic presence of heterointerfaces and the epitaxial NiS nanosheets improves the hydrogen evolution reaction (HER). The onset overpotential of the best ternary catalysts is 35 mV, and overpotentials of 70 and 115 mV are attained by the current densities of 10 and 100 mA cm⁻², respectively. Electrochemical impedance spectroscopy (EIS) studies reveal that the charge transfer resistance reduces remarkably for the best ternary electrocatalyst due to enhanced electron transfer at interfaces. Our findings show that the epitaxial NiS nanosheets increase the active catalytic surface area, synergistically elevate the intrinsic catalytic activity by introducing heterointerfaces, and remarkably support accommodating the H_{ad}. ATTARZADEH, NAVID

Biography of Presenter:

He studied materials science and engineering and continued his education with an MSc. in chemical and materials engineering. He worked for the research institute of the petroleum industry, where he found his interest in energy conversion and eco-friendly new energies. He joined the Center for Advance Materials Research at UTEP to work under the supervision of Prof. Ramana and fulfill his interest and inspiration in hydrogen energy and beyond. He has been the author and co-author of 18 journal



papers with more than 430 citations. He participated in reviewing the manuscripts submitted to prestigious journals, including Electrochimica Acta, Journal of Alloy and Compounds.



Synthesis and Characterization of Pulsed-Laser Deposited Ba(Fe_{0.7}Ta_{0.3})O₃–δ Thin Films

<u>Nolan T. Herbort</u>,^{1, 2} Ramana C.V.^{1, 2*} ¹Center for Advanced Materials Research (CMR), University of Texas at El Paso ²Department of Aerospace and Mechanical Engineering, University of Texas at El Paso

Abstract

Research and development activities in the topical area of semiconducting metal oxides (SMO) for application in a wide variety of sensors for utilization in domestic and industrial sectors is continually rising. The strong, continued interest in SMOs is primarily driven by the increased market size of sensors for consumer and industrial applications. Optimization of industrial processes require rapid sensor responses, and along with these optimizations they reduce the amount of hazardous chemicals being released into the environment from these processes. Recently, Ba(Fe_{0.7}Ta_{0.3})O₃ $-\delta$ (BFTO) has been evolved as an efficient oxygen sensor material with a functionality over a broad temperature and oxygen partial pressure range. However, efforts directed to understand the fundamental scientific aspects of crystal chemistry and phase stabilization, especially as a function of variable thermochemical synthetic conditions, in BFTO materials is meager. In this context, in the present work, we focused our efforts on the synthesis and characterization of bulk and thin film Ba(Fe_{0.7}Ta_{0.3})O₃-δ (BFTO30) materials. The BFTO compounds were synthesized using the conventional high-temperature solid-state chemical reaction method. The structure and phase stability of the BFTO bulk materials studied in order to optimize the bulk target, which was used to fabricate thin films by pulsed-laser deposition (PLD). The BFTO films were made by PLD by varying the deposition temperature and oxygen pressure. The effect of these thermodynamic parameters on the structure, composition, and optical properties is established.

Biography of Presenter

Nolan Herbort is a PhD Student at the University of Texas at El Paso studying Mechanical Engineering. He has a Bachelor of Metallurgical and Materials Engineering from the University of Texas at El Paso. He is currently performing research at the Center for Advanced Materials Research under Dr. Ramana C.V., and has had an internship with the Airforce Research lab in the summer of 2022.





Spin polarization in Iron Oxide Materials for Enhanced Oxygen Evolution Reaction

<u>Aruna Narayanan Nair</u>,¹ Kavish Saini, ¹ Sara E Fernandez, ¹ Mariana Marcos, ¹ Samir A Muniz, ² Srinivasa Rao Singamaneni, ² Dino Villagran,¹ Sreeprasad Sreenivasan^{1*} ¹Department of Chemistry and Biochemistry, University of Texas at El Paso ²Department of Physics, University of Texas at El Paso

Abstract

The performance of various renewable energy devices such as fuel cells, electrolyzers, and metal-air batteries heavily relies on the interconversion of OH/H₂O with a singlet ground spin state without unpaired electrons and O₂ in the spin-triplet state with two unpaired electrons. However, due to the non-conservation of spin, this reaction requires additional energy and exhibits slow kinetics. Hence, it is crucial to consider the "spin transition" in addition to "charge transfer" to achieve a true breakthrough in reducing the high overpotential and increasing the kinetics of oxygen electrocatalysis. Recently, using an external magnetic field to enhance the kinetics of oxygen electrocatalysis has emerged as an advanced strategy. The most significant contribution of a magnetic field to oxygen electrocatalytic reactions is its effect on the spin polarization of the catalysts, resulting in the spin selectivity afforded under the field. While most research has shown spin-regulated oxygen evolution reaction (OER) only on ferromagnetic catalysts, we demonstrate that ferrimagnetic and superparamagnetic samples can also couple with external magnetic fields, enhance OER activity, and the extent of enhancement depends intimately on the total magnetic moment of the catalyst. Different electrochemical and control experiments, including analysis under various temperatures, stirring, and magnetic field orientations, revealed that the magnetic field-induced enhancement in ferrimagnetic and superparamagnetic iron oxide (f-Fe₃O₄ and s- Fe₃O₄) occurs via spin selectivity effects. Thus, this study proves for the first time a positive correlation between the magnetic moment and spin polarization in enhancing the efficacy of OER. This work provides novel perspectives for the design and synthesis of magnetic catalytic materials and opens up new avenues for external magnetic field-enhanced electrocatalysis.

Biography of Presenter

Aruna Narayanan Nair graduated with BS-MS in Physics from Indian Institute of Science Education and Research, Thiruvananthapuram. Currently, she is pursuing her Ph.D. in Chemistry

at the Department of Chemistry and Biochemistry at The University of Texas at El paso. Her research interests include charge and spin modulation in materials for electrochemical energy device applications.





In-situ Magnetically Sensitized Ni-Phthalocyanine-based Covalent Organic Framework and their MXene Heterostructures for Spin Selective Oxygen Evolution Electrocatalysis

Lissette Garcia Enriquez¹, Aruna Nair¹, Kavish Saini¹, Daniel Alejandro Gomez Bustos¹, Sreenivasan Sreeprasad^{*1}

¹Department of Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, Texas 79968, United States

<u>Abstract</u>

Oxygen evolution reaction (OER) is a crucial process in many energy conversion and storage systems, including electrochemical water splitting and zinc-air batteries. Efficient and durable electrocatalysts for OER are required to enhance the performance and sustainability of these systems. In this study, we report the in-situ magnetization of Ni-Phthalocyanine-based Covalent Organic Framework (NiPc-COF) and their MXene heterostructures for spin-selective OER electrocatalysis. The NiPc-COF/MXene heterostructures exhibited enhanced electrocatalytic performance for OER, with a lower overpotential and higher current density than the pristine Ni-Pc-COF and MXene alone. This enhancement is attributed to the synergistic effect of the in-situ conversion of the NiPc spin unit from 0 to 1 in alkaline medium and the conductive nature of MXene. Furthermore, the spin-enhanced performance of NiPc-COF/MXene electrocatalyst was tested in a zinc-air battery. The discharge performance of the zinc-air battery using Ni/Pc-COF/MXene as an air cathode shows an improved discharge capacity and higher power density in a presence of a magnetic field compared to the regular conditions. This work provides a new strategy for designing efficient electrocatalysts for OER, and the spin-selective property may have potential applications in spintronics and magnetic storage devices.

Biography

Lissette Garcia Enriquez graduated in B.S in Chemistry from University of Havana in 2017. Currently she is pursuing her Ph.D. in Chemistry in the University of Texas at El Paso. Her research interests are based on synthesis and applications of sustainable nanotechnology materials. Now she is specializing in atomically tunning of Covalent Organic Frameworks structures for energy generation and storage applications.





Magnetic Single Molecule Catalyst for Electrocatalytic Water Splitting

Kavish Saini,¹ Anju Yadav,¹ Aruna N Nair,¹ Lissette Garcia Enriquez,¹ Shize Yang,² Xin Guo², and Sreeprasad T. Sreenivasan^{1*}

¹Department of Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, TX, 79968 ²Eyring Materials Center, Arizona State University, Tempe, Arizona 85287

Abstract

Water splitting systems rely heavily on the efficiency of the electrocatalytic oxygen evolution reaction (OER), which is a complex and multi-step process involving the conversion of diamagnetic hydroxyl species to paramagnetic oxygen molecules. This spin conversion requires additional energy and often leads to high overpotentials for most OER catalysts. Single atom catalysts (SACs) have emerged as a promising catalyst class due to their high specific singleatom metal sites, versatile coordination design, and efficiency. However, SACs can be prone to deactivation under harsh conditions, reducing their catalytic activity. In this study, we designed a NiCl₂dppp transition metal complex-based single molecule catalyst (SMC) immobilized on graphene acid (GA). In the NiCl₂dpp on GA (NiGA) catalysts, the SMC is stabilized by strong noncovalent interactions, such as H-bonding and pi-pi stacking. The resulting strong interfacial connection and preferential band alignment facilitate efficient electron transfer from NiCl₂dpp to GA, generating highly active interfacial catalytic sites for OER. Further, we identified in-situ structural changes of NiCl₂dppp under highly alkaline conditions, which transformed NiGA into a magnetic spin-active system, that can facilitate spin-polarized OER under an external magnetic field. When exposed to an applied magnetic field (~300mT), the catalyst demonstrated a dramatic change in overpotential, reducing it from 290mV to 270mV at 1mA cm⁻², and increasing the current density by 50%. Our control experiments confirmed spin-dependent OER activity with a low Tafel slope of 52mV Dec⁻¹ for NiGA. The findings suggest that in-situ and ex-situ structural tailoring of SMCs could provide a pathway for magnetically triggered spin-selected OER and water splitting systems.

Biography of Presenter

My name is Kavish Saini and I am currently pursuing my Ph.D. in the Department of Chemistry and Biochemistry at the University of Texas at El Paso. My research primarily focuses on materials chemistry, specifically in the development of electrocatalysts for water splitting devices and qubit materials for quantum computing. I obtained my Master's degree in Chemistry from the Indian Institute of Technology Jodhpur in 2021, where I gained expertise in Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR).





Fabrication and Characterization of High Quality Rutile-Phase GeO₂ Films on MgO(100) for Application in Optoelectronics

<u>Paul Nalam</u>, Debabrata Das, and C.V. Ramana The University of Texas At El Paso

Abstract

Ultra-wide bandgap materials (UWBG) with energy bandgaps ~4eV or larger are currently of immense interest for the development of devices for high-power electronics, deep-ultraviolet (DUV) optoelectronics, energy harvesting, electrocatalysis and quantum information processing. In this context, the functional metal oxide GeO₂ is important for its large bandgap (4.5-6.0 eV), ambipolar dopability and large thermal conductivity. GeO₂ exists primarily in two crystalline polymorphs: the rutile / tetragonal (r) phase and the α -quartz / hexagonal (h) phase. Both polymorphs exhibit interesting and useful optical and opto-electronic properties. However, since it exists in multiple metastable phases with similar formation energies, isolated synthesis of multiple polymorphs with high crystal quality is challenging and has hindered its adoption into advanced optoelectronic applications. Here, we employed radio-frequency magnetron sputtering, which is a relative cost effect method, to deposit r-GeO₂ thin films on MgO (100) substrates in a controlled oxidation environment. The lower degree of interfacial lattice mismatch between r- GeO_2 and MgO enabled to tune the degree of epitaxy of the thin film based on the oxidation environment. The surface morphology, growth mechanism, optoelectronic properties, crystallography, and chemical stoichiometry of these thin films are studied in detail using atomic force microscopy, UV-Vis, Photoluminescence spectroscopy, Ellipsometry, X-ray diffraction, Transmission electron microscopy and X-ray photoelectron spectroscopy.

Biography of Presenter

Paul Gaurav Nalam is currently a Ph.D. student in Prof. C. V. Ramana's lab the Center for Advanced Materials Research, working in the field of Ultra-wide band gap material systems based on GeO₂ thin films. He did his masters in Material science and Data science.





The Electrochemical Performance of Manganese-Oxide Anodes for Lithium-ion Batteries

David Sanchez,¹ Dr. Mataz Alcoutlabi,² Oscar Rivas

¹Department of Mechanical Engineering University of Texas Rio Grande Valley, 1201 W University Drive, Edinburg, Texas 78539, USA

Abstract

Lithium-ion batteries (LIBs) have become of great importance as the 21 century brought many advancements in portable computing, electric vehicles, and other advanced portable electronic devices. The reliance of these devices in addition to the continuous dispersant of greenhouse gases, due to recycling and production of lithium-ion batteries, calls for the advancement of LIBs with high energy density and specific power while minimizing emissions produced as a resultant from mining and manufacturing of rare earth elements. The objective of this study is to evaluate the electrochemical performance of Manganese-oxide (MnO2) short fibers-anode prepared from with $CH_3COO)_2Mn 4H_2O$ precursor fibers. The reason for using MnO2 as anode materials for LIBs is that manganese is less environmentally benign and has a theoretical specific capacity of 1230 mAh g-1 which is higher than that for other metal oxides. The electrochemical performance will be analyzed using galvanostatic charge/discharge and cyclic voltammetry (CV) experiments. The charge/discharge profile of the MnO2 anode showed good electrochemical performance after 100 cycles at a current density of 100 mA g⁻¹. The CV results agree with the charge/discharge experimental results. The MnO2 short-fibers anode delivered a specific capacity of 1090 mAh g-1 at 100 mA g⁻¹ indicating good electrochemical performance.

Biography of Presenter

My name is Oscar Rivas, a senior UG student currently attending the University of Texas Rio Grande Valley for a bachelor's degree in mechanical engineering. I currently work as a research assistant in the battery team in ME at UTRGV that studies the effects of structure and morphology of different metal-oxides on the electrochemical performance of anodes used in lithium-ion batteries. My current academic awards are that have been on the Dean's List since Fall 2020 and was in the Honor's List in Fall 2021.





Production of Piezoelectric Structural Health Monitoring Sensor for Composite Structural Panels on Spacecrafts

Allan Cedillo,¹ Karen Lozano,¹

¹Mechamical Engineering Department, The University of Texas Rio Grande Valley, Edinburg TX 78539

Companies such as Boeing and Airbus have transitioned from alloys to reinforced composites for structural panels on their aircrafts. Significant improvements have resulted from this transition such as weight reduction and improved mechanical/thermal resistive properties. As the positive outcomes of composites are notable, it is of interest to widen the use use of these materials in the aerospace industry. A challenge to overcome relies on the ability to implement Structural Health Monitoring sensors (SHMs) that can withstand harsh environments. The purpose of this project is to develop an SHM sensor to be mounted unto a composite panel and capable of converting it into a smart panel. The SHMs will be used as a form of a Nondestructive Testing technique to provide data on the condition of the component's structure while in service. The SHM sensor will be composed of polyvinylidene fluoride (PVDF) nanofibers blended with polydiacetylene (PDA). The fiber based mebranes will be developed using the Forcespinning® technique. PVDF nanofibers have been reported to possess promising mechanical/thermal properties combined with attractive piezoelectric response, adding the PDA will result in enhnacing the sensing ability by promoting a colorimetric response to applied temperature. This project is ongoing, currently the focus is on optimizing nanofiber production parameters. Multiple parameters are being tested and fibers analyzed using scanning electron microscopy. A compromise among fiber yield, fiber diameter and homogeneity of the system (lack of beads) is being considered during the optimization process. Once the ideal system is developed, thermal, electrical, and mechanical characterization will be conducted on the developed samples and under certain stimuli to evaluate sensing response. As adequate material property data is gathered the integration between the nanofiber system and composite structure will be designed.

My name is Allan Cedillo, I am from McAllen, Texas where I was born and raised. Currently a graduate student at the University of Texas Rio Grande Valley. I acquired my associate degree in engineering sciences at South Texas College on Dec. 2019. Following that, I transferred to UTRGV where I completed my bachelor's degree in mechanical engineering on May 2022 and decided to continue to expand my education with my Master's degree in Engineering Materials. I have a deep passion for material science specially materials that have potential applications in the Aerospace industry. I hope to one day be part of a team of engineers that help make human civilization multiplanetary.





Development and Fabrication of A Bristle Based Constant Flow of Current and Voltage Triboelectric Nanogenerator for Harvesting Rotational Energy

Islam Uddin Shipu,¹ Alejandro Flores², Karen Lozano³, M. Jasim Uddin⁴ ^{1,4}Department of Chemistry, 1201 W. University Drive, Edinburg, TX-78539, USA ^{2,4}Department of Mechanical Engineering, 1201 W. University Drive, Edinburg, TX-78539, USA

Abstract: Triboelectric Nanogenerators (TENGs) have emerged as a promising technology for harvesting energy from the environment. They generate electrical power by converting mechanical energy from the surroundings into usable electrical energy. However, the current output of TENGs is limited, and it is dependent on the frequency of force applied to the device. This limitation has impeded the widespread adoption of TENGs as an energy harvesting solution. To overcome this limitation, a new TENG design based on a bristle structure utilizing Poly Fiber and Horsehair attached to a rotational cylindrical shaped structure has been proposed. The proposed design generates higher current output by using multiple bristles to collect and transfer charges. The device is powered by hand circular motion, and the output voltage and current have been measured up to 8V and 10 µA, respectively. The proposed design shows great promise as a practical and efficient energy harvesting solution. The proposed device has an outer cylinder with a 5.5 cm radius and a height of 14.2 cm. The inner cylinder is 15.2 cm tall and has a radius of 4.5 cm. The bristles of the outer cylinder are 2 cm long and 0.5 cm wide, and the bristles of the inner cylinder are 8 cm long. The constant current and voltage generated by this TENG make it suitable for charging electrical devices. The proposed TENG design is expected to be further tested in efficiency at different speeds and applied to a cup connected to an electrothermal device for cooling. It presents new opportunities for further research and development of TENGs for energy harvesting. UTRGV_Shipu_Islam Uddin_Abstract.

Biography of Presenter:

Islam Uddin Shipu, a driven and accomplished individual, holds a bachelor's degree in chemical engineering and polymer science and is currently pursuing a master's degree in chemistry. Shipu has gained valuable experience working in the field of materials science, specifically in

manufacturing tribo and piezoelectric nanogenerators for energy harvesting and sensing applications. He has also worked as a process engineer in a NaOH production plant in Bangladesh, where he honed his skills in the chemical manufacturing industry. Shipu's dedication and hard work have been recognized through numerous awards, including the welch graduate student scholarship and being named a finalist in the big idea competition 2021, issued by the center for innovation and commercialization (CIC) at the University of Texas Rio Grande Valley.







Enhancement of PTFE-PVA Triboelectric Effect with Multiwall Carbon Nanotubes coating

Fernando Viesca,¹ Diego de León,² PhD. Jasim Uddin ¹ Mechanical Engineering Department University of Texas Rio Grande Valley ² Chemistry Department University of Texas Rio Grande Valley

Abstract

With the increased demand of energy brought by a developing society, an increased need for alternative energy solutions becomes important. Triboelectric nanogenerators (TENGs) have emerged as a promising solution for energy generation in small electronic devices. Improving the surface charge energy is essential to increase the electrical output performance of TENGs. In this study a TENG consisting of Forcespinning® (FS) Polytetrafluoroethylene nanofibers (PTFE-NFs) and Forcespinning® (FS) Polyvinyl alcohol nanofibers (PVA-NFs), as the negative and positive layers respectively, were fabricated. A modification to the PTFE-NFs were made by coating the surface of the PTFE-NFs with multiwall carbon nanotubes to generate higher electrical output. Multiwall carbon nanotubes (MWCNTs) were dispersed in a deionized water solution using three different surfactants: Sodium Dodecyl Sulfate (SDS), Sodium dodecylbenzenesulfonate (SDBS), and Triton X-100 (TX-100), then the dispersions were analyzed. PTFE-NFs were submerged into the dispersion for 24 hours to coat the surface of the NF mat and increase the electrical output, like voltage. A 25.4 x 25.4 mm² PTFE-NFs/PVA NFs TENG device was created by using 3D Stereolithography (SLA) technology, where a simple spring contact separation system was selected. Thin copper foil was used as electrode for both nanofiber mats. PTFE-NFs were characterized using a Scanning Electron Microscope (SEM) and X-Ray Diffraction (XRD). The electrical performance was characterized using an oscilloscope with the addition of a potentiometer.

Biography of Presenter (in 11 Pt Arial Font)

This My name is Fernando Viesca, and I am 25 years old I was born in Mexico in a small city called Saltillo in the state of Coahuila. Since I was a young kid, I was introduced to math and I always wanted to learn how things worked, so when I grew up, I decided that for my bachelor's degree I was going to study materials science engineering. I also finished my degree with a minor in foundry processes, and I completely loved my degree. I worked for 3 years in a company until I decided I wanted to continue studying and start pursuing a master's degree, this is how I end up here in UTRGV chasing a graduate program in mechanical engineering with concentration in materials science.





Improving the Dispersion of Silicon/Silicon Dioxide Quantum Dots

Adriana Chapa,¹ Kristine Q. Loh,² Vivian E. Ferry² ¹Author's affiliation: The University of Texas Rio Grande Valley ²Author's affiliation: University of Minnesota

Abstract:

Through the years there has been a growing need for renewable energy sources, LSCs also known as Luminescent Solar Concentrators, are devices that can generate renewable electricity. LSCs are composed of a transparent *waveguide* and that waveguide is what's coated with a luminescent solution. Silicon Quantum Dots (Si QDs) are semiconductor nanocrystals that broadly absorb UV light and photoluminesce near-infrared light. Si QDs can suit LSC applications as they are nontoxic, are made from an abundant element, and have succeeded in renewable energy technology. We use nonthermal plasma to synthesize Si QDs, but as-synthesized, Si QDs have a high defect density. Silicon quantum dots absorb water and through a span of 3 to 6 months create a silicon dioxide shell. To shorten the creation of the Silica Shell we did a process called high-pressure water vapor annealing, that oxides the plasma synthesized silicon quantum dots and reduced the wait to 3 hours. The silicon dioxide (SiO₂) shell protects the Si QD core and reduces the defect density. Unfortunately, Si/SiO₂ nanoparticles still agglomerate due to the nonpolar silicon hydride and polar silanol surface groups that prevent dispersion in either polar or nonpolar solvents. This work focuses on developing a method for the Si/SiO₂ QDs to stay in a stable, homogeneous mixture. This study varied different aspects of the dispersion by experimenting with various ligands, pH levels, and solvents. We characterized the solutions by using FTIR, UV-Vis, and PL spectroscopies. We concluded that using PEG-Silane as a ligand in an acidic environment with a polar solvent led to a stable, homogeneous mixture with a high photoluminescence intensity.

Biography:

I am a Student at the University of Texas Rio Grande Valley studying mechanical engineering with a minor in chemistry. I have been working since August 2021, for the PREM program working under Dr. Arturo Fuentes and Dr. Horacio Vasquez. My project has focused on electrospinning fibers as well as hybrid ES/FS fibers. My work consists of creating solutions for the production of nanofibers from either electrospinning or hybrid spinning, where I characterize them using various machines such as SEM, rheometer, and FAMAS. I was also able to attend an REU MRSEC at the University of Minnesota Summer of 2022. I worked under Dr. Vivian Ferry on a project

consisting of creating a homogeneous dispersion of silicon/silicon dioxide quantum dots. Programs like PREM motivate my curiosity and excite me to learn new findings on solving world problems.





Biosensing Capabilities of poly(N-isoproylacrylamide) Thermoresponsive Fibrous Hydrogel

Dipasree Bhowmick,¹ <u>Fabian Rodriguez</u>,¹ <u>Valeria Sanchez</u>,¹ Victoria Padilla,¹ Karen Lozano¹ ¹Author's affiliation: University of Texas Rio Grande Valley

Abstract

Temperature responsive hydrogels are broadly studied as smart polymeric gels. These gels have the ability to respond to changes in temperature, and, therefore, are viable candidates for sensing applications. Poly(N-isopropylacrylamide) (PNIPAM) based thermosensitive hydrogels demonstrate great potential in different biomedical and energy applications. As PNIPAM exhibits an abrupt coilto-globule transition around body temperature, 37°C, it is specifically ideal for biomedical applications. The PNIPAM composite hydrogels demonstrate high mechanical strength while being biocompatible and biodegradabile. In this work, PNIPAM/MWCNT composite hydrogel with fast thermal/conductive response and structural integrity is facilely prepared via Forcespinning[™] and subsecuently crosslinked by undergoing heat treatment. N, N'-Methylenebisacrylamide (BIS) was used as a crosslinker agent in order to increase the stability of the fibers and inhibit PNIPAM from dissolving in water. These crosslinked fibers were subsequently processed into fibrous hydrogels in order to increase the surface area of the hydrogel and, therefore, increase the sensing capabilities. This nanofibrous membrane becomes a hydrogel when hydrated at the phase transition temperature (37°C-45°C). SEM analysis demonstrated that the fibrous structure of the nanofiber membrane was maintained within the hydrogel. DSC, TGA and FTIR curves, the crosslinked process can be confirmed. When analyzed on a potentiostat, the fibrous PNIPAM hydrogel exhibits a favorable change in the resistance when heated to the globule phase. This establishes a correlation between the sensor's electrochemical properties and the thermal phase transition. Therefore, this nanofibrous hydrogel sensor demonstarted a good thermal-resistance response which is favourable for biosensing applications.

Fabian Rodriguez

I joined PREM in Spring of 2022. I am currently pursuing a bachelors degree in Mechanical Engineering with a minor in Chemistry. I plan on pursuing a PhD in Material Science/Engineering, or Chemical Engineering. During my time in PREM, I have worked on two projects. The first centered around determining ideal processing parameters to produce nutritionally dense Pullulan nanofibers. The second project I have been apart of has focused on using PNIPAM nanofibers to create a hydrogel biosensor.

Valeria Sanchez

I am currently pursuing a bachelors degree in Mechanical Engineering. In 2019, I worked as an administrative assistant for Scala Consultores. I started working for PREM in Fall of 2022 and have since began collaborating in a project with the purpose of enhancing the properties of a hydrogel biosensor with PNIPAM nanofibers. Aside from my position in PREM, being involved with The Rocket Launchers has allowed me to apply knowledge from my courses hands-on.







Exploring Forcespinning[™] of Ultra-High-Temperature Ceramic Nanofibers

Yazmin Cortes¹, Caleb McCoy¹, Ayla Davila¹, Rogelio Benitez¹ ¹Department of Mechanical Engineering The University of Texas Rio Grande Valley, Edinburg, Tx

Abstract

Several synthesis methods exist for the fabrication of transition metal carbide nanocrystalline nanoparticles, nanorods, nano-powders, and nanowires; however, it is still a great challenge to fabricate long and continuous ultra-high-temperature transition metal carbide nanofibers using scalable techniques for mass production. In this project, novel transition-metal carbide nanofibers are fabricated by the carbothermal reduction of polymer precursor nanofibers manufactured by ForcespinningTm. Solutions consisting of 15 wt. % Ammonium Metatungstate (AMT), 13 - 20 wt.% Polyvinylpyrrolidone (PVP) with a molecular weight of 1,300,000 g/mol, and deionized water were prepared in a scintillation vial and mixed with a magnetic stirrer for at least 24 hours to promote the intimate mixing and spun at fixed angular velocity (4,000 - 9,000 rev/min). Fibers were collected into mats, dried, and crosslinked at 280°C in air for 2 hours and subjected to a carbonizing heat treatment of a range of 600°C - 1000°C with soak times of 60 & 120 minutes in a tube furnace operating under Argon atmosphere. The oxidation behavior of the fibers after exposure to air at high temperatures was also investigated. Their microstructure was studied by SEM after each furnace heat treatment. The fibers will be analyzed using other characterization techniques such as TGA, XPS, and FTIR. The knowledge obtained from this project will enable the large scale fabrication of other ceramic fibers that exhibit a resistance to higher temperatures.

Biographies

Yazmin Cortes was born and raised in Mission, Tx, and is an Undergraduate Mechanical Engineering student graduating Fall 2023 from UTRGV. She joined PREM in 2022 and is currently working under Dr. Rogelio Benitez in the Ceramics Lab. Yazmin joined as a research assistant in January 2022 for research on the spinnability and characterization of ceramic nanofibers. She has plans to attend the UMN MRSEC REU this summer.

Caleb McCoy was born and raised in McAllen, Tx, and is an Undergraduate Mechanical Engineering student graduating Fall 2023 from UTRGV. Caleb began as a research assistant in June 2022 under the direction of Dr. Rogelio Benitez in the Ceramics Lab. His research focuses on the carbonization and oxidation of ceramic nanofibers. Caleb obtained an internship for Material Manufacturing and Aerospace with Janicki Industries for May – September 2023.





Design of Fibrous Membranes for Drug Delivery Application Through Emulsion-Based Systems

Intisar (Zeina) Qubbaj, Cesar Montalvo, Victoria Padilla, Karen Lozano

University of Texas Rio Grande Valley

Abstract

Nanofibers have attractive features to be used as an ideal drug delivery system due to its high surface area to volume ratio, allowing a high encapsulation efficiency and loading capacity. This research explores the feasibility of producing fibrous structures by combining two polymeric phases through an emulsion system for encapsulation of an active component with therapeutic properties, using Forcespinning® technique. Baicalin, a flavone glycoside compound extracted from the root of a traditional medicinal plant named Scutellaria baicalensis (SB), was considered in this study due its extraordinary anti-inflammatory, antioxidant, and antiviral activities. Polyvinyl alcohol (PVA) and Polycaprolactone (PCL) solutions were used as external and internal phases for the emulsion preparation. Three different internal phase concentrations (10, 20, and 30 wt.%) were used to study its influence on the fiber structure morphology. The presence of surfactant (tween 80) and the feasibility of encapsulating Baicalin were also analyzed. Beads on string structures were the predominant morphology obtained by the emulsion-based system, with beads sizes in the range of 2 to 10 µm. The results from the optical microscope and SEM images show there is a distinct correlation between the size of the droplets and beads for all systems. The presence of tween 80 produced smaller droplets diameters, as expected, but the bead sizes increased significantly. Based on the fiber production yield and sample homogeneity, 20% of the internal phase was the emulsion selected for baicalin encapsulation. Through the FTIR spectra were identified the functional groups of the membrane's components. The final membranes were successfully crosslinked, demonstrating water stability with potential to be used in drug delivery application.

Biography of Presenters

Cesar Montalvo:

I am a mechanical engineering undergraduate and currently a junior. I joined PREM in Spring 2021, and since then I have been able to learn from many talented people by working alongside them. Overall, my experience with research in PREM has been very enriching to my academic career, being surrounded by a culture of hard-work and dedication has definitely steered me in the right direction for the future. **Zeina Qubbai:**

I am an undergraduate in mechanical engineering and am currently a junior. I started working with PREM-UTRGV in the summer of 2022 and was able to have the opportunity to join this project. My experience with research has been very positive and I enjoy the process of trial and error, since through this I have developed skills for testing different nano-composite properties and following important experimental procedures.





Improved Nanofiber Morphology Control & Higher Production Yield Through Electro-Centrifugal Spinning

<u>Carlos A. Delgado</u>,¹ Dr. Arturo Fuentes,² Dr. Horacio Vasquez ^{1, 2} University of Texas of Rio Grande Valley

Abstract

An experimental setup for Electro-Centrifugal Spinning (ECS), relatively novel method of creating nanofibers, was created to take advantages of the benefits of both Electrospinning (ES) and Centrifugal Spinning (CS). The project seeks to maintain the high CS nanofiber production yields, while additionally incorporating ES benefits such as high alignment, fine diameter, and low variability of overall diameters. Initial tests using an Electro-Centrifugal Spinning (ECS) machine were conducted using PEO and DI H₂O. SEM characterization of the produced fibers with different processing parameters (e.g., rotational speed and electric field voltage) are presented. Initial ECS experimental results show great potential for improved nanofiber morphology control and higher production yields.

Biography of Presenter (in 11 Pt Arial Font)

Born in Hidalgo, Texas, and raised for most of his childhood in Reynosa, Tamaulipas Mexico. Carlos Alberto Delgado is an active graduate researcher working at PREM in UTRGV, he attained a Bachelor of Science in Mechanical Engineering and is currently working towards a Master Degree of Science in Mechanical Engineering.





Graphene Reinforced PVDF Nanofibers Fabricated by the ForceSpinning® Method for Water Desalination Applications

Elmmer A. Vera Alvarado,¹ Md. Abdur Rahman Bin Abdus Salam,² Karen Lozano,³ Ali Ashraf,⁴ ¹University of Texas Rio Grande Valley, PREM ²University of Texas Rio Grande Valley ³University of Texas Rio Grande Valley, PREM ⁴University of Texas Rio Grande Valley

Abstract

Direct contact membrane distillation (DCMD) is a thermally driven energy and cost-efficient desalination technique where low-grade energy from solar or waste heat from plants can be used to recover fresh water from high saline water. Polyvinylidene fluoride (PVDF) nanofiber membranes were prepared by the ForceSpinning® (FS) method, these were later dip coated in different concentrations of graphene-acetone solutions. The ForceSpinning® method, unlike electrospinning, operates in the absence of electromagnetic fields, solely based on the use of centrifugal spinning where nanofiber production is mainly controlled by the angular velocity applied to the spinneret containing the polymer solution or melt. The use of FS method also results in a considerably high yield in a short amount of time. A 0.75 wt.% graphene-acetone solution showed adequate dispersion and distribution on the developed PVDF nanofiber membrane as confirmed by Scanning Electron Microscopy (SEM). The graphene-coated nanofiber membranes underwent a heat treatment process to reduce the probability of pore wetting during testing, while also ensuring the integrity of the PVDF nanofibers. Both coated and uncoated membranes were studied to evaluate the effect on mechanical strength and permeating flux. Water contact angle and surface roughness varied depending on the percentages of graphene in the coating solution. For the uncoated membrane, the contact angle was 130° and the coated one had 140°. At 58°C, the brine side concentration was 8000 ppm and for 50 ml of fresh water, tests were run for 210 min and 285 min for uncoated and coated membrane respectively. The salt rejection was 97.5% and 93.5% respectively for the coated membrane and uncoated membrane whereas the permeate flux was 6.06 Lm-2h-1 and 8.25 Lm-2h-1. Stainless steel filtering wire cloth of 165*1400 mesh size with 6% opening was used to support the PVDF membrane, this membrane presented a clog of approximately 94%. For correction, permeate flux should be nine times the tested one, 54.54 Lm-2h-1 and 74.25 Lm-2h-1. Future testing will be conducted with different support materials with higher porosity. This study presents a promising platform for moderate to high salinity rejection, as well as produced water desalination.

Biography

Born and raised in Matamoros, Tamaulipas, Mexico, Elmmer A. Vera Alvarado decided to pursue a career in Engineering, obtaining a bachelor's degree in Mechanical Engineering at the University of Texas Rio Grande Valley, and in process of acquiring a master's degree in Mechanical Engineering with a concentration in Materials Science at the same institution. He is a member of the Partnership for Research and Education in Materials Science (PREM), and currently operates as a research assistant working under Dr. Ali Ashraf and Dr. Karen Lozano. Vera finds an interest in preserving natural resources and green technology, focusing his research on water purification methods.





Enhancement of PTFE-PVA Triboelectric Effect with Multiwall Carbon Nanotubes Coating

<u>Diego de León¹</u>, Fernando Viesca², PhD. Jasim Uddin ^{1,2} University of Texas Rio Grande Valley

Abstract

With the increased demand of energy brought by a developing society, an increased need for alternative energy solutions becomes important. Triboelectric nanogenerators (TENGs) have emerged as a promising solution for energy generation in small electronic devices. Improving the surface charge energy is essential to increase the electrical output performance of TENGs. In this study a TENG consisting of Forcespinning® (FS) Polytetrafluoroethylene nanofibers (PTFE-NFs) and Forcespinning® (FS) Polyvinyl alcohol nanofibers (PVA-NFs), as the negative and positive layers respectively, were fabricated. A modification to the PTFE-NFs was made by coating the surface of the PTFE-NFs with multiwall carbon nanotubes to generate higher electrical output. Multiwall carbon nanotubes (MWCNTs) were dispersed in a deionized water solution using three different surfactants: Sodium Dodecyl Sulfate (SDS), Sodium dodecylbenzene sulfonate (SDBS), and Triton X-100 (TX-100), then the dispersions were analyzed. PTFE-NFs were submerged into the dispersion for 24 hours to coat the surface of the NF mat and increase the electrical output, like voltage. A 25.4 x 25.4 mm² PTFE-NFs/PVA NFs TENG device was created by using 3D Stereolithography (SLA) technology, where a simple spring contact separation system was selected. Thin copper foil was used as electrode for both nanofiber mats. PTFE-NFs were characterized using a Scanning Electron Microscope (SEM) and X-Ray Diffraction (XRD). The electrical performance was characterized using an oscilloscope with the addition of a potentiometer.

Biography

Diego de Leon is an undergraduate student from The University of Texas Rio Grande under the Department of Chemistry and Department of Manufacturing and Industrial Engineering degree. His previous work relates to algae growth for oil production, flexible nanofiber incorporated with liquid crystals, and nanofiber triboelectric nanogenerators. Diego's goal is to continue his research work and achieve a PhD in material engineering.





Production yield study of pullulan fibers obtained by means of centrifugal spinning. I - Optimization of experimental parameters

<u>Cesar Benitez</u>, Ever Acosta, Martin Lopez, Joseph Casas, Jefferson Reinoza, Karen Lozano The University of Texas Rio Grande Valley (UTRGV)

Abstract

Pullulan, a polysaccharide produced from starch by the Aureobasidium pullulans fungus, has been widely used as an additive in cosmetology, pharmacology, food industry, medicine, among others. This polymer has certain properties that allow it to be used in the production of coatings, films, and fibers, which has generated great interest thanks to its high biocompatibility and degradability properties. Pullulan fibers have been produced by several experimental methods, mainly by Electrospinning technology, which produces high homogeneity degree fibers; however, this procedure can transform only a few mL/h of a polymer solution into fibers, which is guite slow for the growing demand for this material. On the other hand, the Forcespinning technology, consisting of spinning a polymer solution when it is expelled in a jet form by centrifugation, has been able to produce pullulan fibers at a rate of g/min, representing a great advantage in terms of production/time ratio. Investigations related to pullulan fibers production have been based mainly on the feasibility of obtaining composite materials using pullulan as a support for other substances, nevertheless no reports have been found on studies about fiber production of this substance considering different experimental conditions such as the polymeric solution concentration, rotational velocities and humidity in the centrifugation spinning process. In this work, a systematic study of the production yield of pullulan-based fibers, considering the aforementioned experimental variables, was developed. In addition, the polymeric solutions used were rheologically analyzed to determine the relationship between the fiber production performance at different rotational velocities (rpm) and their rheological properties. Some systems achieved production yields close to 90%. Scanning electron microscopy (SEM) and thermogravimetric analyses (TGA) were performed to determine the effects produced in the fibers obtained at different rpm.

Biography:

Cesar Benitez, I am an Undergraduate Mechanical Engineering student graduating in the spring of 2024. Born in Hidalgo, Tx, raised in Reynosa, Tamaulipas Mexico. I joined PREM in September 2022 working under the direction of Dr. Reinoza in the nanofiber lab. I am planning

to attend the UMN MRSEC REU this summer.



Jefferson Reinoza, I am a professional in chemistry. Master's degree in chemistry related to Enhance Oil Recovery by thermocatalytic processes. Ph.D. degree in photosynthesis of porous polymeric materials with selective absorbent properties. Currently in a postdoctoral

position at UTRGV, in the College of Engineering and Computer Science/Center for Nano Technology department, under the supervision of Dr. Karen Lozano.





Energy Harvesting with Thermoplastic Polyurethane Nanofiber Mat Integrated with Functionalized Multiwalled Carbon Nanotubes

Julia Salas,^{1,2} Dr. M. Jasim Uddin,^{2,3} Dr. Karen Lozano.^{2,4}

¹Photonics and Energy Research Laboratory, University of Texas Rio Grande Valley, Edinburg, Texas 78539, United States.

²Department of Mechanical Engineering, University of Texas Rio Grande Valley, Edinburg, Texas 78539, United States.

³Department of Chemistry, University of Texas Rio Grande Valley, Edinburg, Texas 78539, United States. ⁴Center for Nanotechnology, University of Texas Rio Grande Valley, Edinburg, Texas 78539, United

States.

Abstract (in 11 Pt Arial Font)

In recent years, triboelectric nanogenerator (TENG) has been received great attention to fabricate flexible and stretchable energy harvester that can convert mechanical energy to electrical energy. This paper studied poly(vinylidene fluoride) (PVDF) and thermoplastic polyurethane (TPU) nanofiber membranes based flexible TENG. Both PVDF and TPU nanofiber (NF) triboelectric functional layers were synthesized by Forcespinning (FS) technique. To improve the performance of the TENG, the TPU NFs were decorated with multiwalled carbon nanotubes (MWCNT) that are functionalized with fluorine, amide, and carboxylic groups with variable time (6, 12 and 24 hours) of exposure and concentration. The TPU nanofibers demonstrated a stronger interaction with the carboxylic functionalized multiwall carbon nanotube (c-MWCNT) as depicted by its electrical performance when compared to the non-modified fibers. The maximum open circuit voltage (Voc) recorded at a 4 Hz hand tapping frequency for modified TNEG was ~252 V, which 152% higher than basic TPU/PVDF TENG. Furthermore, the c-MWCNT functionalized TPU/PVDF TENGs were evaluated with varied compressive force applied by a pneumatic cylinder and the maximum alternating voltage and current outputs were obtained of 158 V and 170 µA at 30 psi pressure. To demonstrate the potential of harvesting human motion into charging small electronic device, the modified TENG showed that it can charge 3.03 V connected with 1 µF capacitor by hand tapping motion at 4 Hz load frequency for only 25 seconds, suggesting the prospect of our as fabricated TENG has the capability as self-charging flexible energy harvester.

Biography of Presenter (in 11 Pt Arial Font)

Julia I. Salas obtained her B.S. in Civil mining engineering, in the University of Talca, Chile in 2020, after this she obtained her M.S. in mechanical engineering in the University of Texas Rio Grande Valley, in 2021. Her research interest mainly are in energy harvesting devices and how to functional polymers for this objective





Color tunable aerogels/sponge-like structures developed from fine fiber membranes

<u>Alexa Villarreal</u>,¹ Raul Barbosa,¹ S, Bose, B, Srivastava,¹ V. Padilla, ¹ A. Abraham, ¹ A. Portales, ¹ and K. Lozano¹

¹ Mechanical Engineering Department, University of Texas Rio Grande Valley, 1201 W. University Dr., Edinburg, Texas 78539

Abstract

Aerogels are solid, lightweight, and highly porous materials. Their solid porous 3D network structure, high specific surface area, low density, and unique chemical, thermal and optical properties make them suitable candidates for a variety of applications in the fields of catalysis, energy storage, and sensors. Herein this work, the development of macroscopic aerogels from 1D systems, such as nanofibers, has resulted in a novel pathway to obtain porous and lightweight architectures. Bright green, red, and tunable color emitting aerogels were obtained with luminescent nanofibers as the precursor system. A simple, low cost, and environmentally friendly process is followed where luminescent fillers are encapsulated within fibers which were subsequently freeze-dried to form 3D aerogels and sponge-like structures. Moreover, the aerogels/sponge-like structures show higher photoluminescence intensity than the fiber mats due to an increase of porosity which provides higher and direct interaction with the fillers and therefore an efficient light absorption resulting in higher luminescence. Manganese doped zinc germanate (Mn: Zn₂GeO₄) nanorods and chromium doped zinc gallate (Cr: ZnGa₂O₄) nanoparticles were used as the source of green and red emissions respectively. By precisely adjusting the stoichiometric ratios of nanorods and nanoparticles within the nanofibers, a broad spectrum output is obtained from the final aerogels. We foresee that these types of photoluminescent aerogels have promising potential applications in a variety of fields such as display devices, solidstate lighting, sensors, etc.

Biography of Presenter

Alexa Villarreal is a mechanical engineering, with a concentration in material science, graduate student engaged in research under the supervision of Dr. Karen Lozano at the University of Texas Rio Grande Valley. Her research focuses on the synthesis and study of polymer based nano fiber materials for a variety of applications such as biomedical, filtration, sensors, and more.

Experienced in organizing and presenting multiple research posters at National and International research conferences. As well as actively participated in collaborations with other Universities to increase productivity, research findings, and networking. Co-author and co-first author, of multiple published articles that have helped further personal knowledge, training and understanding of the research experience and expectations.





Electrostatic Potential of hBN Moiré Superlattices

Dong Seob Kim^{1,2}, Rigo Mayorga-Luna³, Dingyi Ye⁴, Tixuan Tan⁵, Yue Ni^{1,2}, Zhida Liu^{1,2}, Roy C. Dominguez³, Mitchell Ford³, Frank Y. Gao^{1,2}, Saba Arash^{1,2}, Kenji Watanabe⁶, Takashi Taniguchi⁷, Suenne Kim⁸, Chih-Kang Shih^{1,2}, Keji Lai^{1,2}, Wang Yao⁵, Li Yang⁴, Xiaoqin Li^{1,2}, and Yoichi Miyahara^{3,9} ¹Department of Physics and Center for Complex Quantum Systems, The University of Texas at Austin, Austin, Texas, 78712, USA. ²Center for Dynamics and Control of Materials and Texas Materials Institute, The University of Texas at Austin, Austin, Texas, 78712, USA. ³Department of Physics, Texas State University, San Marcos, Texas, 78666, USA. ⁴Department of Physics, Washington University in St Louis, St. Louis, MO, 63136, USA. ⁵Department of Physics, and HKU-UCAS Joint Institute of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China. ⁶Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan. ⁷International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan. ⁸Department of Photonics and Nanoelectronics, Hanyang University, Ansan, South Korea. ⁹Materials Science, Engineering and Commercialization Program (MSEC), Texas State University, San Marcos, Texas, 78666, USA.

Abstract

Twisted hexagonal boron nitride (hBN) layers have been demonstrated to exhibit ferroelectric domains due to charge redistribution at the interface. Here, we investigate the electrostatic potential at the top surface of twisted hBN bilayers, prepared by folding exfoliated thin flakes. Using Kelvin Probe Force Microscopy measurements, we show that this potential can be engineered by tuning the twist angle and adjusting the thickness of the top hBN layer. Furthermore, we study double moiré superlattices with different twist angles at each interface. These findings can be further extended to twisted multilayers to significantly expand the versatility of hBN and moiré superlattices in engineering material properties.

Biography of Presenter

Graduate student at UT Austin since 2019. Work on new moiré physics in twisted hBN.





Quantum coherence of new quasi-particles in a doped semiconductor monolayer

<u>Yue Ni</u>,¹ Di Huang,^{1,2} Kevin Sampson,¹ Kenji Watanabe,⁴ Takashi Taniguchi,⁴ Jesper Levinsen,³ Meera M. Parish,³ Dmitry K. Efimkin,³ and Xiaoqin Li,^{1,*}

¹ Department of Physics and Center for Complex Quantum Systems, The University of Texas at Austin, Austin, TX, 78712, USA.

² MOE Key Laboratory of Advanced Micro-Structured Materials, Shanghai Frontiers Science Center of Digital Optics, Institute of Precision Optical Engineering, and School of Physics Science and Engineering, Tongji University, Shanghai 200092, China

³ School of Physics and Astronomy and ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Monash University, Victoria 3800, Australia

⁴ Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Abstract

Since the discovery of graphene, Van der Waals (vdW) materials have become one of the central in condensed matter physics. These layered materials are strongly bounded within twodimensional plane but weakly bound to adjacent layers by van der Waal forces. Therefore, it is possible to achieve few layers or even monolayer by exfoliation from bulk forms. This makes it feasible to create various van der Waal heterostructures which provide a wide platform to exploit the novel properties of these materials. Transition metal dichalcogenides (TMDs) are semiconductor vdW materials that exhibit strong light-matter interaction, large excitonic oscillator strength and binding energies, and unique spin-valley locking by optical selection rules. This proposed dissertation will use two-dimensional coherent spectroscopy (2DCS) as the tool to explore the quantum coherent dynamics of exciton and other excitonic charge complexes in TMDs monolayer and bilayer in order to advance the understanding of the underlying physics in optoelectronic properties of these materials which is necessary for the future study in Van der Waals heterostructures.

Biography of Presenter (in 11 Pt Arial Font)

Yue Ni is a fifth-year graduate student in the Physics Department at the University of Texas at Austin. He received his Bachelor's degrees in Physics and Mathematics from Stony Brook University.

Yue's research is fouced on the light-matter interaction in the nanoscale semiconductors using various optical spectroscopies. He has gained extensive experience in device fabrication of two-dimensional materials and optical system building, especially in Ultrafast Two-dimensional Coherent Spectroscopy (2DCS).





Mechanism of Atom Rearrangement upon Thermal Annealing in BGa(In)As

<u>Q. Meng</u>¹, R.C. White¹, R.H. El-Jaroudi¹, T. Dey², S.R. Bank¹, M.A. Wistey^{2,3} ¹Microelectronics Research Center and ECE Dept., The University of Texas at Austin ²Materials Science, Engineering, and Commercialization Program, Texas State University ³Physics Dept., Texas State University

Abstract

The incorporation of the physically small boron atoms into conventional III-V alloys provides a method for strain engineering of near-infrared, direct-bandgap alloys that can be lattice-matched to silicon and other substrates. The advantage of incorporating boron, compared with more highly mismatched alloys (HMAs), is a larger predicted solid solubility, suggesting that less degradation of material properties can be expected with the incorporation of boron. However, B-III-V remains underexplored in both theory and experiment. While HMAs often suffer from poor optical properties as-grown, thermal treatment can often successfully recover the optical properties though it is typically accompanied by an undesirable blueshift in emission/absorption wavelength. This blueshift and improvement in photoluminescence (PL) have been observed with thermal annealing of molecular beam epitaxy (MBE) grown BGaInAs films; however, no blueshift is observed from BGaAs films. We investigated the effects of atomic rearrangement on the electronic and optical properties of B-III-V alloys to understand this dichotomy using density functional theory (DFT) with hybrid functionals performed on the Texas State LEAP Cluster. We found an increase in bandgap with increasing numbers of B-In bonds, along with more favorable system energy, suggesting that In atoms tend to be in the first nearest neighbor position of B under thermally-stable conditions. In contrast, the calculated bandgap differences, and energetic driving force due to B-B rearrangements were much smaller, suggesting BGaAs alloys are not likely to show a strong blueshift upon annealing. We found that the short-range effect from localized B limited the bandgap change with B-B rearrangement while local strain compensation between B and In brought a larger effect on the bandgap. Additionally, we found the intrinsic matrix element strength of BGaInAs increased with increased B-In bonds, contributing to a portion of the improvement in optical quality. Since improvements in PL intensity were observed from both BGaAs and BGaInAs films, we suspect the removal of the defects plays a significant role. Studies of the mechanism of B-In rearrangement and In concentration on the magnitude of blueshift in BGaInAs are in progress.

Biography of Presenter

Qian Meng is a Graduate Research Assistant in the Microelectronics Research Center and the Electrical and Computer Engineering Department at the University of Texas at Austin. She is co-advised by Prof. Seth Bank and Prof. Mark Wistey. She received her B.S. degree from Sichuan University and M.S. degree from the University of Texas at Austin, both in Electrical Engineering. Her research interests include understanding the fundamental properties of highly mismatched alloys (HMAs) grown by molecular beam epitaxy (MBE).





Tunable Orthogonal Reversible Covalent (TORC) Bonds:

Reconfigurable Nanoparticle Networks and Molecular Assemblies

Diana L. Conrad¹, Taylor N. Bell¹, Christopher D. Wight¹, Stephanie A. Valenzuela¹, Hannah S. N.

Crory¹, Jiho Kang²

Thomas Truskett², Delia Milliron², and Eric V. Anslyn¹ ¹Department of Chemistry, University of Texas at Austin ²Department of Chemical Engineering, University of Texas at Austin

Abstract

Linker-mediated colloidal gel assembly of nanocrystals can be controlled by the dynamic covalent reactions of ligands and linkers. Specific examples of dynamic covalent reaction pairs, known as tunable orthogonal reversible covalent (TORC) pairs, are thermodynamically stable, yet kinetically labile, and uniquely exhibit no cross-reactivity in the presence of other functional groups. In this work TORC functionalities are incorporated within sequence-controlled peptide strands, utilizing solid state peptide synthesis (SSPS) and copper catalyzed click chemistries, thus creating ligands that will bind to the surface of nanocrystals. Linkers are organic molecules containing the corresponding TORC functionality, which bind to the ligands and create networks of nanocrystals. The TORC-peptide components have been individually designed to promote solubility, favorable cross-linking, and attachment to nanocrystals or surfaces; ultimately delivering control over the molecular assembly and tunability of the resulting material.

Biography of Presenter: Diana Conrad

Diana Conrad is a second-year graduate student at the University of Texas at Austin, co-advised by Professors Eric Anslyn and Delia Milliron. Her research with MRSEC investigates the optimization of TORC chemistry for the synthesis of TORC functionalized ligands and linkers and the study of pH-controlled linker-mediated colloidal gel assembly of nanocrystals.





PEDOT Laden Hydrogels for Light Mediated Controlled Release

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Abstract

This project focuses on the utilization of a previously explored hydrogel crosslinking system in collaboration with the Betancourt lab at Texas State University. The hydrogel system in questions utilizes a reversibly-covalently crosslinked hydrogel with a reversible conjugate acceptor mechanism. Previous research has demonstrated these hydrogels to be viscoelastic, and the equilibrium for this reaction is sensitive to changes in temperature. The other components of this system are poly(ethylene dioxythiophene) (PEDOT) nanoparticles, which release heat when exposed to near-IR light. By combining these two systems, we demonstrate that light can be used as an effective means to control the temperature, and thus the equilibrium, of the crosslinking reaction within the hydrogel. The changes to the crosslinking reaction lead to changes in the hydrogel architecture and material properties. These changes are characterized through UV/VIS spectroscopy and small angle oscillatory rheology. Furthermore, these hydrogels exhibit self-healing properties, and the release of an encapsulated protein can be controlled through the pulsatile exposure of the hydrogel to near-IR light. This hydrogel system demonstrates a promising framework for further research into its use as an injectable, controlled therapeutic delivery system.

Biography of Presenter

Thomas FitzSimons is a post-doc in chemical engineering in the Rosales lab. He received his B.S in chemical engineering at the University of Colorado at Boulder along with a minor in biomedical engineering, and he receives his doctoral degree in chemical engineering from the University of Texas at Austin. His past research topics include photodegradable hydrogels for progenitor neuron cells, stretchable liquid crystal foams, and viscoelastic hydrogels for tissue engineering and drug delivery. In general, his research interests include the combination of chemistry, materials, and polymer science in order to research advances in the field of biomaterials. One of his most important goals is to mentor younger scientists while creating a scientific environment that is accessible and open to everyone.





The Importance of Morphology on Ion Transport in Single-Ion Copolymer Electrolytes: Experiments and Simulations

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Abstract

Single-ion conducting polymer electrolytes (SICPEs) offer high lithium transference numbers and desirable physical properties while maintaining moderate conductivities. Bottlebrush and combbranched copolymer electrolytes are a particular architecture that offer modularity and increased ion solvation. Despite this promise, the ion transport in these systems is poorly understood. In this report, we investigated lithium-ion transport in comb-branched SICPEs using a combination of experiments and atomistic simulations. A series of solvent-free SICPEs were synthesized by copolymerization of poly(ethylene glycol) methyl ether acrylate (PEGMEA) with varying lithiated anionic groups in different ratios of the ionic species to the PEG side chain. Poly(Lithium 3-[(trifluoromethane) sulfonamidosulfonyl]propyl methacrylate-co-poly(ethylene glycol methyl ether acrylate)) (p(MPTFSI-co-PEGMEA) exhibited both highest ionic con- ductivity (on the order of 10⁻⁵ S/cm at room temperature) and degree of decoupling of ionic conductivity from polymer segmental dynamics. Simulations revealed that in electrolytes with low ion concentrations, Li+ transport occurs through the vehicular co-diffusion of lithium ions and the polyanions. In contrast, for higher anion compositions, the primary mechanism of Li+ transport is through Li+ ion hopping among the percolated ionic aggregates. Finally, we demonstrate that the behavior of ion hopping is influenced in a nonintuitive manner by the anion site morphology based on SIPCE anion identity.

Biography of presenter

Zach Brotherton is a second year graduate student in the McKetta Department of Chemical Engineering. He received his B.S. in chemical engineering from North Carolina State University in 2019. As an undergraduate, Zach studied the deposition morphology of stimuli-responsive microgels. Zach joined the Lynd polymer research group shortly after starting study at the University of Texas at Austin. He is studying polymer synthesis for incorporation in advanced composite electrolyte materials. Zach is also interested in the longterm storage of cells and tissues through cryopreservation. In his free time, Zach is an avid sports fan and enjoys cooking Texas-style barbecue.





Wafer-Scale Si-Based Metal-Insulator-Semiconductor Photoanodes for Water Oxidation Fabricated Using Thin Film Reactions and Electrodeposition Shang-Hsuan Wu', Soonil Li', and Edward T. Yu'*

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<u>Abstract</u>

Photoelectrochemical (PEC) water splitting is a promising technology for converting solar energy into clean and storable chemical energy. In PEC cells, semiconductors play a key role in absorbing photons from the light source to create mobile charge carriers. Various semiconductor materials have been studied for high-performance PEC cells, including metal oxide, nitrides, Si, III-V compound semiconductor materials. Among these, Si-based photoelectrodes have drawn much attention due to its moderate bandgap, high charge mobility, long carrier diffusion length, cost effectiveness, and scalability in manufacturing. To improve the stability of Si-based PEC cells in operation, metal-insulator-semiconductor (MIS) structures have been widely employed. In this work, we employ a simple and highly scalable method to fabricate high-performance, extremely stable Si-based MIS photoanodes and demonstrate its application to the fabrication of wafer-scale photoanodes. Localized conduction paths formed via an Al/SiO₂ thin-film reaction enable lowresistance charge extraction even through thick insulating layers, and this approach has been shown in our previous work to yield photoanodes with excellent stability. In addition, we demonstrate a two-step Ni/NiFe electrodeposition process to create efficient OER catalysts. The Ni/NiFe catalyst allows for a high Schottky barrier between Si and Ni, lowering the photoanode onset potential, while the NiFe surface layer improves catalytic performance. A wafer-scale photoanode is combined with the commercially available poly-Si solar cell array to produce a zerobias water splitting system under AM 1.5G sunlight simulator or outdoor illumination.



Quantum Emitters from Strained WSe₂ Monolayer

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and Edward T. Yu¹

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Abstract

Strain engineering is a powerful tool that strongly influences electronic structure and exciton states in 2D transition metal dichalcogenides (TMDs). Among TMDs, WSe₂ has gained attention as a host for quantum emitters due to its intrinsic ground exciton state—a lowest-lying dark exciton state that hybridizes with defect levels upon strain, giving rise to bright single photon emitters. In particular, the application of uniform biaxial tensile strain to monolayer WSe₂ causes a downshift of the conduction band minima at K and K' valleys which then hybridize with states within the band gap that originate from point defects in WSe₂ such as Se vacancies. This hybridized state allows optical transitions of long-lived dark excitons which are otherwise forbidden for unstrained WSe₂ due to spin and momentum conservation. The high oscillator strength, increased charge and spin lifetime, and long diffusion length of dark excitons allow them to store and transport quantum and classical information which could be beneficial for quantum information processing, sensing, and secure communications. Therefore, the ability to manipulate the emission of dark exciton states is crucial for the design of future quantum emitters based on strained monolayer WSe₂.

Recent advances in spatially localized quantum emitters based on strained WSe₂ utilize strain fields created via transfer of monolayer WSe₂ to prefabricated dielectric nanopillars, metal nanoparticles, etched trenches or holes, or through precise nanoindentation techniques using atomic force microscopy. However, the above-mentioned methods provide low quantum emitter yield due to monolayer piercing, random and uncontrollable quantum emission, limited substrate effects, and restrictions in operating conditions. To realize high purity and tunable quantum emitters, it is necessary to have controllably strained WSe₂ devices operating at cryogenic temperatures. In this study, we demonstrate control of dark exciton dynamics of suspended WSe₂ monolayers via electrostatic deflection at cryogenic temperatures. Our technique implements strain fields which are generated by applying a bias voltage between a suspended WSe₂ monolayer and an electrode in a back gate geometry. Since the monolayer WSe₂ is grounded and the back gate is positively biased, an electrostatic force is induced between the two surfaces, which in turn results in the deflection of the suspended WSe₂ monolayer membrane. Experimental results revealed a significant monolayer deflection of ~50 nm at 15V gate bias at 300K, corresponding to ~0.23% biaxial tensile strain. Moreover, photoluminescence measurements at 7K showed a \sim 20 meV shift of dark exciton emission peak from 1.67 eV (0V) to 1.65 eV at (30V). corresponding to approximately 0.2% biaxial tensile strain assuming a redshift of all exciton peaks at a rate of 95meV/%. This strain value is lower than our theoretical result (0.6% strain at 30V) which could be attributed to the change in mechanical constants and built-in strain at lower temperatures. This dark exciton emission shift is an essential step towards the development of controllable WSe₂-based quantum emitters that can be integrated into various optoelectronic systems.



Electric field tunable hybridization in MoSe2 bilayers

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Abstract

Transition metal chalcogenide (TMD) monolayers and twisted bilayers have been extensively investigated with most studies focusing on unique exciton resonances and correlated insulator states. Many effects observed in twisted bilayers are also present in natural bilayers, which is a much simpler system less susceptible to inhomogeneity introduced by a variety of factors. However, existing researches on natural bilayer are mainly focused on stark effect while the trions and excitons hybridization remains undiscovered. Here, we study a dual-gated MoSe2 natural bilayer using optical reflectivity measurement and discover the distinct properties of trions (bound electron-hole pairs). Since natural bilayer has an indirect band gap, that the vallance band (VB) of Γ point is higher than K point without or under little electric(E) field, thus extra holes will occupy Γ point first and bond together with the exciton in K valley. However, K valley can be tuned up higher than Γ point by E field. With a hole doping level inside the intrinsic region, that when only a few holes are doped into the system, by tuning the E field, the VB of K will be shifted higher than Γ , leading to a transformation from $\Gamma - K$ valley momentum indirect trions to K valley momentum direct trions. Since the direct trions are harder to form, the resonance under high E field is weaker than that of low E field. After overcoming the Schottky barrier, injected extra holes enhanced trion resonances in both cases. Our result shows that E field over a critical point opens a new channel of momentum direct trions other than momentum indirect trions, along with a larger formation difficulty revealed by the position and strength of the resonances. The trion signal shows strong layer hybridization, which is tunable by electric field due to band alignment tuning.

Biography of Presenter

Xiaohui Liu finished her bachelor's degree in Zhejiang University, China. Now she works in Dr. Xiaoqin Elaine Li group, mainly focusing on optical resonances in TMD materials. She is able to fabricate gated-samples and perform optical measurements, such as PL and absorption on it. She is also learning the 2D coherent spectroscopy, which is a unique tool to investigate the nonlinear dynamics in materials.





Chiral Phonons in a Quantum Magnet CoTiO₃

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Abstract

The interplay of charge, spin, and lattice degrees of freedom in correlated materials often leads to complex and fascinating properties. Recent developments have brought new perspectives to collective excitations, e.g. the topological nature of bosons. For example, inelastic neutron scattering experiments revealed non-trivial band topology for both magnons and spin-orbit excitons in CoTiO3. Here, we report intriguing phonon properties resulting from a combination of strong spin-orbit coupling, large crystal field splitting, and trigonal distortion in this quantum magnet. Specifically, the interaction between spin-orbit excitons and phonons endows chirality to two Eg phonon modes observed in the magneto-Raman spectra with large phonon magnetic moments. The remarkably strong magneto-phononic effect originates from the hybridization of spin orbit excitons and phonons due to their close proximity in energy. While chiral phonons have been associated with electronic topology in some materials, our work suggests new opportunities may arise by exploring chiral phonons coupled to topological bosons.

Biography of Presenter:

David Lujan is a Ph.D. graduate student in Xiaoqin (Elaine) Li's research group at the University of Texas at Austin. He received his bachelor's degree from Texas A&M University –

College Station. He studies magnetic bilayers and van der Waals using optical spectroscopy techniques. Measuring magnons and their dispersion allows one to reveal fundamental material properties and microscopic interactions such as DMI. He has been using inelastic light scattering techniques (e.g.) Raman spectroscopy and Brillouin light scattering, and magneto-optical Kerr effects to investigate fundamental excitations and control of phases of matter.

