Program Overview

Friday, October 27, 2023

10 AM – Noon: Meeting of the NYSS APS Executive Committee

1:00 – 1:30 PM: Registration

Session I: CIMS Conference Room, Louise Slaughter Hall (SLA)

Welcome Remarks: 1:30 – 1:45 PM

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<th>1:45 – 2:30 PM</th>
<th>Next Generation Photovoltaics: The Hot Carrier Solar Cell</th>
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2:30 – 3:15 PM: Theory-guided Discovery of New Superconductors

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3:15 – 4:00 PM: Novel Approaches to Photovoltaic and Photonic Power Conversion

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<td>Prof. Seth Hubbard, Rochester Institute of Technology</td>
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------- Poster Setup, CIMS Conference Room: 4:00 – 4:15 PM-------

Session II: CIMS Conference Room, Louise Slaughter Hall (SLA)

4:15 – 5:15 PM: Poster Viewing, Networking, etc.

5:15 – 6:00 PM: Dinner

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<th>6:00 – 7:00 PM</th>
<th>Keynote talk: Synchrotron X-ray Facilities: An Introduction and Applications to Energy Research</th>
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<td>Prof. Joel Donald Brock, Cornell University</td>
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7:00 – 7:15 PM: Best Poster Prize Announcement

See next page for Saturday, October 28 program details
Saturday, October 28, 2023

Coffee, Networking, Breakfast: CIMS Conference Room, Louise Slaughter Hall (SLA)

Session III: CIMS Conference Room, Louise Slaughter Hall

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<th>Time</th>
<th>Topic</th>
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<td>9:00 – 9:40 AM</td>
<td>Solar Power for Solar Probe</td>
<td>Dr. Geoffrey A. Landis, NASA John Glenn Research Center</td>
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<td>9:40 – 10:20 AM</td>
<td>Multi-electron Redox for Na-ion Batteries</td>
<td>Prof. Hao Liu, SUNY Binghamton</td>
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<td>10:20 – 10:40 AM</td>
<td>Coffee Break</td>
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<td>10:40 – 11:20 AM</td>
<td>Agrivoltaics: Photovoltaics and Agriculture Synergy</td>
<td>Prof. Santosh Kurinec, Rochester Institute of Technology</td>
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<td>11:20 AM – Noon</td>
<td>Introduction to Solid-state Batteries and the Pathway to Anode-free Architecture</td>
<td>Prof. Howard Qingsong Tu, Rochester Institute of Technology</td>
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<td>Noon – 12:30 PM</td>
<td>Boxed lunch</td>
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CIMS Conference Room
Building 74A (78)
Conference Location
Keynote Speaker

K1. Synchrotron X-ray Facilities: An Introduction and Applications to Energy Research

Author: Prof. Joel D. Brock

Affiliation: School of Applied and Engineering Physics (A&EP), Cornell University

Abstract: Modern synchrotron facilities provide unique techniques for studying the structure and behavior of matter at the microstructural, molecular, and atomic levels. The Cornell High Energy Synchrotron Source (CHESS), a ring-shaped synchrotron, 768 meters in circumference and 5 stories underneath the Cornell University campus, delivers highly collimated x-ray beams over a billion times more intense than a conventional laboratory source to 7 experimental stations. These experimental stations each have unique instrumentation, opening new research vistas in condensed-matter physics, materials research, structural biology, chemistry, geology, structural and functional materials, and cultural heritage. In this talk, I will give a brief introduction to synchrotrons, synchrotron-based x-ray techniques at CHESS, and a few of the broad scientific applications. I will then focus in on recent energy research at CHESS on fuel cells and batteries. I will conclude with tips on how to access CHESS’s capabilities.

Bio: Joel Brock is the Given Foundation Professor of Engineering in A&EP at Cornell University and currently serves as Director of the CHESS. Professor Brock got his B.S. in Physics from Stanford and did his Ph.D. with J. David Litster and a post-doc with Robert J. Birgeneau (both at M.I.T.). He joined the A&EP faculty in 1989. He was a NSF Young Investigator from 1992-97. He is a member of the graduate fields of Applied Physics and Materials Science & Engineering. He served as Director of Graduate Studies for the Graduate Field of Applied Physics from 1993-99. He served as Director of the School of Applied & Engineering Physics from 2000-2007. He became Director of CHESS in 2012. He currently serves on: the International Advisory Committee (IAC) for the RIKEN SPring-8 Center, Japan; the IAC for the National Synchrotron Radiation Research Center (NSRRC), Taiwan; the External Advisory Committee for the National High Magnetic Field Laboratory, Tallahassee; and, he chairs the Scientific Advisory Committee for the Stanford Synchrotron Radiation Lightsource (SSRL) at the SLAC National Accelerator Laboratory. In addition to CHESS, Brock is affiliated with the Cornell Center for Materials Research (CCMR), the Center for Alkaline-Based Energy Solutions (CABES), and the Cornell Energy Systems Institute (CESI). He is a Faculty Fellow of the Cornell Atkinson Center for Sustainability and is a Fellow of the American Physical Society.
**Invited Speakers**

**I1. Next Generation Photovoltaics: The Hot Carrier Solar Cell**

**Authors:** Prof. Ian R. Sellers

**Affiliation:** Department of Electrical Engineering, University at Buffalo SUNY

**Abstract:** To enable the large-scale implementation of solar cells for utility scale energy applications, improvements in power conversion efficiency and system cost reductions must be achieved. To circumvent the fundamental limitations of single energy gap solar cells, devices based on third generation processes have been proposed. In this presentation I will briefly introduce the operational principles of the solar cell and the limitations of current technology. This will be followed by a discussion of potential concepts to overcome losses in such devices with particular emphasis on the so-called hot carrier solar cell, a protocol which has been proposed to circumvent the particularly parasitic thermalization losses in photovoltaic systems and therefore increase the power conversion efficiencies of such technologies.
I2. Theory-guided Discovery of New Superconductors

Author: Prof. Alexey Kolmogorov

Affiliation: SUNY Binghamton

Abstract: Recent discoveries of record-breaking superconducting materials represent major breakthroughs in fundamental research and put the century-old dream of creating room-temperature superconductors critical for emerging technologies within grasp. As further search for practical superconductors demands exploration of vast chemical spaces, modeling has been playing an increasingly important role in guiding the experimental effort. In this talk, I will describe key strategies developed in the Physics and Materials Science communities for finding new conventional superconductors from first principles and will present examples of predicted and confirmed materials based on light elements\[^{1-4}\]. I will also overview our on-going development of machine learning methods capable of accelerating the search for new synthesizable materials\[^{5,6}\].

\[^{5}\] Module for Ab Initio Structure Evolution (2009-), http://maise-guide.org
\[^{6}\] Kharabadze et al., NPJ Comput. Mater. 8, 136 (2022)
**I3. Novel Approaches to Photovoltaic and Photonic Power Conversion**

**Author:** Prof. Seth Hubbard

**Affiliation:** Rochester Institute of Technology, NanoPower Research Laboratories

**Abstract:** There is an ever-growing demand for increased power and sophistication in the satellite systems orbiting our planet, driven in part by increasing reliance on high speed communication and data links. Photovoltaics conversion is one avenue that can be explored to meet these challenges, in space as well as terrestrially, with III-V’s being the most promising materials for very high efficiency devices. This talk will give an overview of PV research at RIT, discussing our quantum well multi-junction approach and specific results using superlattices and various light management schemes. I will also discuss our work on a new type of three-terminal, monolithically integrated device that combines both power generation and optical communication. Our recent results show the capability for either photovoltaic or photonic power conversion (using both GaAs and InP based systems) combined with electro-absorptive modulation of data signals at 1.55 µm for simultaneous free space optical communication and energy production.
Solar Power for Solar Probes

Author: Dr. Geoffrey A. Landis

Affiliation: NASA John Glenn Research Center

Abstract: The sun is the closest star to the Earth, and by far the most important—but many features of the sun remain mysteries. To learn about these mysteries, NASA’s ambitious Parker Solar Probe mission has flown closer to the sun than any mission in history, reaching a temperature of 2,500 degrees F as it approaches to within 9 solar radii of the surface of the sun. But how do you power a mission that flies right into the corona of the sun? Dr. Landis will talk about the challenges the mission was designed to overcome, and how we powered a mission to the edge of the sun.
I5. Multi-electron redox for Na-ion batteries

Author: Prof. Hao Liu

Affiliation: Department of Chemistry, SUNY Binghamton

Abstract: The charge storage capacity of battery cathode materials is governed by the number of electrons transferred per redox center. Most intercalation-based electrodes are based on one-electron transfer per transition metal ion center, which limits their theoretical capacity. Enabling multi-electron transfer per transition metal ion center could potentially multiply the charge storage capacity of electrode materials. While intercalation compounds with multielectron redox have been demonstrated for Li-ion batteries, few cases have been reported for Na-ion batteries. We have explored a couple of silicate- and phosphate-based materials for their activity for multi-electron redox. A multitude of structural, spectroscopic, and electrochemical methods were used to elucidate their reaction mechanisms. The intercalation of the larger Na ions induces substantial structural rearrangement to accommodate the multi-electron redox reaction, which offers new opportunities for the development of high-capacity battery materials.
I6. Agrivoltaics: Photovoltaics and Agriculture Synergy

Author: Prof. Santosh K. Kurinec

Affiliation: Electrical & Microelectronic Engineering, Rochester Institute of Technology

Abstract: Agrivoltaics (Agri-PV) is defined as a land-use concept that co-locates photovoltaic (PV) energy generation with agriculture and nature conservation, which are dependent on sunlight. Agri-PV presents an opportunity to maximize land use efficiency while promoting eco-friendly energy generation and agricultural productivity. Agri-PV installations should guarantee that the agricultural activity is at least preserved, and at most improved. An approach of PV implementation on farmland in harmony with agriculture and nature conservation, needs to be at the core of Agri-PV development and that is where scientists, engineers and farmers need to learn from each other. Certain skills and knowledge are needed to further accelerate the deployment of Agri-PV. The talk will present the design of PV systems that involve panel configurations such as monofacial fixed-tilt modules suspended above agriculture, monofacial single-axis modules fitted with trackers which alter their angle throughout the day, and vertical bifacial modules set in fence-like rows. The configurations are based on the type of crops grown for optimal land use, and an increase in land productivity. Beyond that, PV modules can provide shading and shelter in dry climates to make irrigation and water retention easier, fostering more vibrant ecosystems beneath them. Crops beneath or adjacent to panels can also increase their efficiency by cooling the system through transpiring water vapors. Future trends on transparent PV and the integration of artificial intelligence (AI) and machine learning (ML) for planning & monitoring system performance will also be introduced.
I7. Introduction to solid-state batteries and the pathway to anode-free architecture

Author: Prof. Howard Qingsong Tu

Affiliation: Rochester Institute of Technology

Abstract: Li-metal solid-state batteries are the holy grail for the next-generation rechargeable battery technology due to their improved safety and energy densities. The anode-free architecture for solid-state batteries (AFSSB) is an emerging structure to reduce the cost of handling Li-metal foil and further increase the volumetric and gravimetric energy densities. Adding a buffer layer (BL) between the current collector (CC) and the SE seems a promising strategy to tackle the remaining issues in AFSSB (such as dendrites growth and low Columbic efficiency). However, except for several preliminary trials reported at the laboratory scale, there is no research yet on the systematic investigations of the AFSSB architecture with a BL, let alone proposing an optimized design/prototype for this new structure. An optimized design should be mainly focused on the innovation at the anode side, including the selection of BL material (usually contains Li-alloyable metals and matrix material) and the pairing CC and SE material, the control of BL microstructure (porosity, particle size, and weight ratio), and the treatment of BL interfacial properties (surface adhesion, charge-transfer, etc.) with the CC and the SE. We apply our data-simulation-experiment approach to find out the optimized design for the AFSSB with BL. The house-developed approach brings together multi-scale simulations, data processing, mechanical design, and experimental efforts.
**Poster Presentations**

**P1. Pt-Ni-Ru Nanoframes with Superior Performance For the Electro-Methanol Oxidation Reaction**

*Author:* Kira Shulman  

*Affiliation:* Binghamton University

**Abstract:** Direct Methanol Fuel Cells (DMFCs) are promising devices for energy conversion with relatively low carbon emissions. However, the sluggish kinetics of the Methanol Oxidation Reaction (MOR) limit the efficiency of the anode and prevent commercialization of DMFCs. Platinum (Pt) is the current standard catalyst for MOR, yet has proven to be both expensive and inefficient. Pt-based alloys with open structures are promising alternatives with the potential to boost MOR, making them more cost-effective. This study reports Pt-Ni-Ru nanoframes (NFs) generated by simple galvanic replacement with outstanding MOR activity due to the synergic effect of alloying and nanoframing. The Pt-Ni-Ru NFs exhibited 2.8 and 2.0 times higher mass and specific activities than the commercial Pt/C catalyst, respectively. The stability of the Pt-Ni-Ru NFs will also be evaluated and presented. This study demonstrates not only that Pt-Ni-Ru NFs are a strong candidate catalyst for the anode reaction in DMFCs, but also the utilization of open nanostructures and alloying in the production of next-generation catalysts.
Advancements in Anode-Free Solid-State Batteries for Sustainable Energy Storage

Authors: Imtiaz Ahmed Shozib, Dr. Howard Tu

Affiliation: Rochester Institute of Technology

Abstract: In comparison to traditional lithium-ion batteries, solid-state batteries (SSBs) have the potential to provide higher energy density while also being safer and lasting longer. When compared to other types of SSBs, the anode-free architecture stands out due to their more compact design and cheaper processing without the need for lithium metal thin film. This poster discusses the latest advances and developments in anode-free solid-state batteries and highlights their key advantages and challenges.

In this presentation, we focus one of the major challenges on cathode active material (CAM) loading in the composite cathode. Composite cathode for SSBs is typically made up of the CAM, the solid electrolytes (SEs), and carbon. The composite can be fabricated in multiple ways, among which the “simple mixing + high-pressure sintering” approach is the most common method. However, because of the requirement for large SE fraction (30–50 wt.%) for sufficient ionic diffusion, the volume fraction of cathode (CAM loading) and the energy density of current SSBs is low. This work emphasizes the utilization of SEs and CAM to enable the balance between lithium-ion transport and lithium storage. We will showcase various strategies employed to optimize materials and fabrication processes to achieve higher energy density. By reducing SE particle size and increasing the CAM particle size, over 50 vol% cathode active material loading with high cathode utilization can solve this problem and enhance the energy density.
P3. Interfacial Transport of Colloidal Nanoparticles in Porous Media

Author: Hunter Heineman

Affiliation: Rochester Institute of Technology

Abstract: Nanoparticle transport in porous media is a subject of growing interest, a result of an expanding nanomaterial industry and an increased concern about nanoparticles as environmental contaminants. Despite extensive investigations probing the factors affecting transport in porous media, interfacial clustering in the partially saturated regime remains mostly unexplored. To investigate the clustering at fluid-fluid interfaces, we fabricate two-dimensional porous media models using microfluidics. We use a fluorescent microscope to image the transport and retention of fluorescent nanoparticles as they flow through our micro-model porous media. Image analysis, along with bulk material measurements, allow us to determine the concentration and spatial distribution of retained nanoparticles. We see that retention is greatest at fluid-solid interfaces. This retention is observed to alter local fluid flow.
P4. Unexpected Fingering Instabilities in Reactive Transport in Porous Media

Authors: William Braun, Shima Parsa

Affiliation: (1) Kate Gleason College of Engineering, (2) College of Science, Rochester Institute of Technology

Abstract: Reactive transport in porous media occurs in a wide range of applications including carbon dioxide sequestration and battery membranes. Precipitation of solute often gives rise to geometric modifications of the porous network, ultimately impacting the transport properties of the medium. Hence, it is crucial to understand the balance of reaction, advection, and diffusion for a stable system. To investigate the formation and transport of precipitates we use polymer solution-antisolvent interactions in a microfluidic porous medium. Using optical microscopy, we observe antisolvent interactions with a polymer solution at different concentrations. We observe anomalous fingering phenomena at antisolvent-polymer solution interfaces which are not present in non-reactive and miscible fluid-fluid interfaces.
P5. Understanding and Predicting High-Tc Superconductivity in Metal Borocarbides

Authors: Charley R. Tomassetti, Gyanu P. Kafle, Edan Marcial, Igor I. Mazin, Elena R. Margine, and Aleksey N. Kolmogorov

Affiliation: (1) Department of Physics, Applied Physics, and Astronomy, Binghamton University-SUNY, (2) Department of Physics and Astronomy and Quantum Science and Engineering Center, George Mason University

Abstract: For application in widespread technologies, superconducting materials must be mass produced and operate at temperatures above the boiling point of liquid nitrogen (> 77 K). A delithiated form of the bulk LiBC material comprised of honeycomb BC layers was previously predicted to superconduct at 100 K, supplanting the record-holding $T_c = 40$ K of ambient-pressure MgB$_2$ conventional superconductor. After two decades, Li$_x$BC has never been observed to superconduct despite extensive experimental effort. This work investigates a range of disordered Li$_x$BC morphologies to explain the superconductivity suppression in this intriguing compound. We propose that Li$_x$BC re-intercalation with select alkali and alkaline earth metals could lead to synthesis of otherwise inaccessible Li$_x$M$_y$BC materials with high superconducting $T_c$. 
P6. Studying the Properties of Niobium Oxide

Authors: Sean Lannon, Scott Lewis, Karsten Beckmann, Nate Cady, Matthew Sullivan, Zachary Robinson

Affiliation: (1) Department of Physics, SUNY Brockport, (2) College of Nanoscale Science and Engineering at SUNY Albany, (3) Department of Physics, Ithaca College

Abstract: Niobium oxide is a strong candidate for implementation into neuromorphic computer technology. The purpose of this research is to develop niobium oxide thin-film synthesis and modification so that the material can be better understood and eventually incorporated into next-generation computers. In particular, we studied the ambient conditions required for the as-deposited amorphous material to undergo crystallization, which is required for realization of the neuromorphic electrical properties. We developed a tube furnace system with a regulated inflow of gas and various vacuum pumps at the exhaust, so that we could control the temperature, pressure, and gas-type during anneals. We used pressures ranging from 10⁻⁶ Torr up to 800 Torr and temperatures ranging from 800 °C to 1000 °C. We also used two types of gas, argon gas and a nitrogen/hydrogen mixture. The samples were then measured using microscopic image analysis and Raman spectroscopy. We have found that the samples underwent the most crystallization at higher pressures and higher temperatures. Crystallization only took place when using the nitrogen/hydrogen mixture, and we had a 0% crystallization rate using argon gas. No crystallization occurred in any samples below 900°C and between the pressure range of 10⁻⁵ Torr and 100 Torr. The only samples to fully crystallize were at atmospheric pressure (760 torr) and 1000°C. Partial crystallization was observed at 900°C in atmospheric conditions.

Authors: Andrew M. Lyon¹ and Santosh K. Kurinec²

Affiliation: (1) School of Chemistry & Materials Science, (2) Electrical & Microelectronic Engineering, Rochester Institute of Technology, Rochester, NY, USA

Abstract: To reduce the emissions of carbon dioxide (CO₂), substitutes for fossil fuel energies with renewables such as wind and solar (PV) are being deployed. The emission factor in electricity generation using fossil fuels is specified by the US Environmental Protection Agency (EPA) as 0.709 Kg CO₂ /kWh. Photovoltaics electricity generation does not emit CO₂. However, CO₂ is emitted during its fabrication, installation, and end of life recycling. A carbon payback time (CPBT) is defined based on these factors. Estimation of lifetime CO₂ emission reduction in using a PV system depends on many factors that include the location of use, and where and how the solar panels are manufactured. In this study, an analysis of annual CO₂ emission reductions from a photovoltaic installation at Rochester Institute of Technology, located in Rochester, NY is conducted. The data on power generation leading to CO₂ offset and the solar panel production (CO₂ emission) was collected and analyzed. Utilizing the EPA emission factor, it has been estimated that the system electricity production offset was 3,097,931 kg of CO₂ in a year. A CPBT of 1.45 years and an energy payback time (EPBT) of 3.08 years are determined. The public is generally familiar with the absorption of CO₂ by plants, so a useful metric for consideration and public communication is to compare avoided emissions to the number of trees needed to sequester that carbon. Based on the EPA Greenhouse gas equivalencies calculations, the RIT PV system generating 4,369,437 kWh in 2022, avoiding 3,097,931 Kg of CO₂ emissions corresponds to 51,632 in equivalent trees planted to capture that associated carbon emission.
P8. Catalytic Dimethyl Ether (DME) Steam Reforming By Density Functional Theory (DFT)

**Authors:** Jason Richards\textsuperscript{1}, Dr. Claire Yang\textsuperscript{2}, Dr. Anjana Talapatra\textsuperscript{2}

**Affiliation:** (1)Department of Mechanical Engineering, University of Rochester, (2)Department of Materials Science, Los Alamos National Laboratory

**Abstract:** Dimethyl ether (DME) is, by many performance and cost metrics, the best multipurpose renewable fuel and hydrogen carrier. DME boasts a hydrogen gravimetric capacity of 13 wt.% and a volumetric capacity of 87 kg H\textsubscript{2}/m\textsuperscript{3}. With its high hydrogen storage capacity and suitability as a hydrogen carrier, DME holds great potential in supporting the hydrogen economy. Recent experiments have enabled the development of a novel core-shell catalyst structure, Cu/CeO\textsubscript{2}/zeolites, as a micro-reactor to improve hydrogen selectivity and yield from DME-steam reforming. For simulation trials, the student used The Vienna ab initio Simulation Package (VASP) and other data analysis and plotting packages for density functional theory (DFT)-based calculations for the DME-steam reforming process. This process involved running simulation trials using these three different catalysts(CuO/CeO\textsubscript{2}/zeolites) and DME to analyze the H\textsubscript{2} and CO\textsubscript{2} product efficiency and the DME conversion efficiency. Running a structural optimization calculation along with a DFT+U calculation of a CeO\textsubscript{2} reaction with DME resulted in finding an optimized lattice parameter of 5.4653 Å and 5.4979 Å. Both of these results are similar to each other and are consistent with the previously reported experimental and theoretical values. With hydrogen selectivity and yield, the hydrogen yield of the reaction increased as the ratio of steam to DME increased. Similarly, the DME conversion yield increased as the ratio of steam to DME increased. The hydrogen yield also increased with an increase in temperature during the reaction.
**P9. Impact of Medium Wettability on Directional Flow based on Immiscible Displacement in Porous Media**

**Authors:** Amir Ibrahim, Shima Parsa

**Affiliation:** Rochester Institute of Technology

**Abstract:** Controlling flow in microfluidic devices where small fluctuations can trigger a cascade of unprecedented events is a challenging task in experiments. Based on concepts of capillary displacement in porous media, we study the formation of a natural valve that consists of asymmetric porous structures. We form a porous medium using a lattice of pillars to achieve a “geometric” valve. This valve enables partial or complete disruption of flow of an invading fluid (water) in one direction while still allowing flow in the opposite direction at the same pressure. Previous simulations suggest a strong valving effect over a considerable range of capillary numbers. Here, we control the wettability of the medium and study the applicability of this geometrical valve for different physical conditions experimentally. Our results show a strong effect of medium wettability on valving between water and air even at small capillary numbers. We observe a hydrophobic medium can effectively impede fluid flow offering opportunities for energy-efficient flow regulation.
P10. Leveraging Soft Matter Chirality for Advanced Materials Engineering

Authors: Michael Grant, Brennan Fingler, Natalie Buchanan, Poornima Padmanabhan

Affiliation: Microsystems Engineering, Department of Chemical Engineering, Rochester Institute of Technology, Rochester, NY

Abstract: Chirality, which refers to the asymmetry, or handedness of molecules can have profound impacts on the properties and behavior of soft materials. This intrinsic feature of organic substrates has been leveraged for numerous applications such as helical self-assembly, circularly polarized luminescence, liquid crystal technology and drug delivery. Yet, while significant improvements in materials within these domains has been reported, a lack of fundamental understanding is present which hinders the rapid exploitation of chirality, retarding novel material discovery within this field. For example, when the polypeptoid block of a poly(n-butyl acrylate)-b-polypeptoid block copolymer is made completely chiral, a decrease in the temperature of the ordered-disordered transition (ODT) is observed. Contradicting this is the report of an increase in the ODT when the poly(lactic acid) (PLA) block of a polystyrene-b-PLA is made completely chiral. Thus, diverging thermodynamics are present with no quantitative rationale for these phenomena warranting a more in-depth mechanistic understanding. Therefore, we employed free energy calculations in conjunction with conformational analysis within particle-based simulations to probe how chirality impacts the disordered phase. We found that traditional theories within polymer physics is unable to capture the helical contributions of these semiflexible chiral polymers, and that pitch, which is unique to these helical structures is the major driving force behind divergent thermodynamics. With fundamental insights regarding the disordered phase quantified, investigations of ordered morphologies are underway, which could lead to enhanced core understandings of chiral block copolymer self-assembly, ultimately expediting the development of novel advanced materials.
**P11. Simulations of Optical Modules in IceCube-Gen2**

**Authors:** Waly M. Z. Karim, Segev BenZvi

**Affiliation:** University of Rochester

**Abstract:** The IceCube Neutrino Observatory is capable of detecting high-energy astrophysical neutrinos from unknown sources as well as bursts of MeV neutrinos produced by galactic core-collapse supernovae (CCSNe). The next-generation telescope, IceCube-Gen2, will encompass nearly ten times the volume as IceCube, and will use multi-PMT Digital Optical Modules (mDOMs) and Wavelength-shifting Optical Modules (WOMs) currently being developed and tested. The design of the new modules will have a significant impact on the sensitivity of IceCube-Gen2 to supernova neutrinos. To estimate the sensitivity and optimize the sensor design, we developed a comprehensive GEANT4 based simulation of mDOMs and WOMs including depth-dependent ice properties surrounding the modules. Currently, it is possible to simulate signal events using positron and electron flux from supernovae neutrinos and background events due to radioactive decay of trace elements inside the detector. The simulations give insight into the performance of the new optical module designs, and can be used to optimize Gen2 to be more sensitive to CCSNe MeV neutrino bursts.
P12. Modeling Chiral Chain Conformations

Authors: Natalie Buchanan and Poornima Padmanabhan

Affiliation: Rochester Institute of Technology

Abstract: Chirality exists at different length scales including molecular, conformational, and phase chirality. In the past decade or so, chiral block copolymers have been self-assembled to form novel chiral phases with many promising applications. However, it is still unclear how chirality effects the thermodynamics of self-assembly, which makes it difficult to identify viable systems for a broad range of applications. Here, we study the interplay between the chiral chain conformation and the overall phase structure using molecular dynamics. First, we developed a model to simulate single chiral polymer chains. The parameters can be tuned to match experimental polymer systems and can capture a large range of chain conformations. Next, we expand our system to look at chiral block copolymers self-assembled into the achiral lamellar phase. The simulations are analyzed to extract measurement of both individual chains as well as the phase as the whole. We find that chirality itself does not dictate the interplay between the length scales; rather the chain conformation itself dictates the effects. This insight can better inform the targeting of polymer systems that will create desirable chiral phases.
P13. Oxygen vacancy formation at misfit dislocations in CeO\textsubscript{2}/SrTiO\textsubscript{3} heterostructures

Authors: Kurt Dawson\textsuperscript{1}, Pratik P. Dholabhai\textsuperscript{2}

Affiliation: (1)Department of Microsystems Engineering, (2) School of Physics and Astronomy, Rochester Institute of Technology

Abstract: Owing to high ionic conductivity at low temperatures, mismatched oxide heterostructures show remarkable promise as electrolyte materials for solid oxide fuel cells, wherein misfit dislocations impact interfacial ionic transport. The effect of misfit dislocations on oxygen ion conductivity in these materials is not fully understood however, and previous studies have shown both enhancement and reduction of ionic conductivity in the presence of misfit dislocations. We will discuss results obtained using first principles density functional theory study of oxygen vacancy defect formation at misfit dislocations in CeO\textsubscript{2}/SrTiO\textsubscript{3} heterostructures. Primary focus will be on predicting interface stability as well as atomic and electronic structure of oxygen defects and extended defects. Presented results include the minimized interfacial structure, Burger's circuit analysis of misfit dislocations, formation energies of dopant-vacancy complexes, favorability of dopant migration to the interface, and charge properties. Interface formation was found to be favorable for both interface terminations, and vacancy formation energy was found to be dependent on interface termination and site. The study ultimately seeks to qualitatively understand how misfit dislocations form at heterointerfaces and their impact on oxygen ion diffusion through the material, with a goal of uncovering trends in material properties that may guide future work into heterostructured oxides and allow more rapid development of superior electrolyte materials.

We acknowledge support from NSF CAREER Award DMR-2042311.
**P14. Radioisotope Thermoradiative Cell Power Generator**

**Authors:** Andrew L. Schaefer, Dr. Seth Hubbard, Dr. Geoff Landis, Dr. Steve Polly

**Affiliation:** Rochester Institute of Technology

**Abstract:** In this project, the feasibility of a thermoradiative cell (TRC) for use to power outer solar system satellite missions is demonstrated. Most space missions utilize photovoltaic arrays to generate their required power, but there are many places in the solar system where sunlight is scarce. As a result, other means of power generation are required. Currently, satellites are equipped with a Radioisotope Thermal Generator (RTG), a large unit that uses the decay of a radioisotope to generate heat which is converted to electrical power using thermoelectric devices. Much of this heat energy is radiated into space through bulky cooling fins. A TRC is able to collect and convert more of this heat energy and radiate away losses itself instead of using a large cooling apparatus. A TRC is a novel semiconductor device that can generate electrical power using any heat source, such as a radioisotope. A TRC works similarly to a solar cell operated in reverse where heat is the input instead of light, and photons are emitted as a byproduct of the power generation mechanism. This device is predicted to exceed the power conversion efficiency of state-of-the-art thermoelectric devices currently used for deep space power systems. While ideal calculations have high efficiencies there are non-idealities that will reduce power generation and efficiency. The power and efficiency are calculated for ideal cases and including non-ideal losses. Losses from non-idealities are generally converted into heat, which in most applications is a total loss. Since a TRC uses heat as the input some of this heat energy may be reclaimed.

Authors: Katelynn Fleming, Dr. Steve Polly, Dr. Seth Hubbard

Affiliation: Rochester Institute of Technology

Abstract: Laser power beaming (LPB) is a wireless power transmission method which sends power via a laser beam traversing from a power station to a specially tuned photovoltaic device a distance away, where it is turned back to electricity. This method allows power to reach hostile regions where it is difficult to lay wires and makes it possible to create temporary or flexible power grids such as from a ship to the shore, or into a natural disaster zone. We develop the photovoltaic device, a laser power converter (LPC), out of In0.20Ga0.80As grown metamorphically on GaAs via metal organic vapor phase epitaxy (MOVPE). The LPC is tuned for a 1064 nm laser, because lasers at this wavelength have already attained high power and coherence, making them suited for long-distance transmission. To withstand a high power density laser while maintaining high efficiency conversion to electricity, we split the device into two vertically stacked LPCs in a two junction (2J) structure, each absorbing half of the incident laser light. The junctions are connected by a tunneling junction, which must be able to pass high current densities while imposing minimal voltage loss. This poster reports on our recent progress toward a 2J LPC by building a 1J LPC and various types of tunneling junctions to connect the two subcells. We report on several different material, structural and dopant combinations.
P16. Memristors and NbO$_2$ Planetarium Show

Authors: Scott Lewis$^1$, Sean Lannon$^1$, Karsten Beckmann$^2$, Nate Cady$^2$, Matthew Sullivan$^3$, Zachary Robinson$^1$

Affiliation: (1)Department of Physics, SUNY Brockport, (2)College of Nanoscale Science and Engineering at SUNY Albany, (3)Department of Physics, Ithaca College

Abstract: Niobium Oxide (NbO$_2$) is a material being studied as a potential candidate for memristors, an electronic device that could be used in conjunction with transistors to improve the processing power, energy efficiency, and memory density of our computers. The goal for this project was to create a planetarium show that showcases the research being done on NbO$_2$. For the show to truly portray the research being done, Blender, a computer animation software, was used to create images to give an in-depth explanation of the research. The show walks through the stages of synthesizing NbO$_2$ and how it will be used in our devices. The show is expected to be viewed by approximately 800 people at the SUNY Brockport planetarium. The process of creating NbO$_2$ begins with sputter deposition, a process in which solid Niobium is bombarded by Argon ions to react with oxygen to make a thin film of Nb$_2$O$_5$. The Nb$_2$O$_5$ is then annealed in a tube furnace, heating it up to temperatures between 800 and 1000 °C to turn it into NbO$_2$. Raman spectroscopy is then used to verify that the material is NbO$_2$. Once we have the NbO$_2$ we can then implement it into volatile memristors, a device capable of neuromorphic computing that can help improve the energy efficiency of our current technology.
**P17.** Computational determination of the solvation structure of LiBF$_4$ and LiPF$_6$ salts in battery electrolytes

**Authors:** M.D. Hashan C. Peiris, Manuel Smeu

**Affiliation:** Materials Science and Engineering, Binghamton University

**Abstract:** Advances in lithium-ion batteries have been significant since their discovery, yet the increasing demand for energy storage necessitates further refinement. This study employs first-principles computational models to explore the interactions between a typical electrolyte solvent mixture, ethylene carbonate (EC) and dimethyl carbonate (DMC), and two lithium salts, LiPF$_6$ and LiBF$_4$. Utilizing ab initio molecular dynamics, we examine the formation and evolution of solvation shells around these salts. Density functional theory is used to assess the energy required to displace and assemble individual solvent molecules from the solvation structures gathered from the trajectories. Both salts exhibit similar interaction energies and solvation geometries, favoring interactions between Li$^+$ ions and carbonyl or ether oxygens, and between BF$_4^-$ or PF$_6^-$ anions and methyl or methylene groups. Notably, our results indicate that the solvation shell surrounding LiPF$_6$ is more readily desolvated than that around LiBF$_4$, suggesting more favorable kinetics and diffusion characteristics.
P18. Computational Modeling of the Reaction Mechanisms in Sulfur Batteries

Authors: Sihe Chen, Manuel Smeu

Affiliation: Binghamton University

Abstract: Energy storage has become one of the most important topics in the field of green energy production. With the rise in renewable energy generation, the demand for high-energy-density batteries is also increasing to match storage needs. Conventional intercalation-based lithium-ion batteries are reaching a performance ceiling in terms of energy density and face problems with dendritic plating behavior and scarcity of source materials. Unlike intercalation-based batteries, conversion batteries release energy by breaking chemical bonds on the cathode side, rather than inserting ions into a crystalline cathode. Sulfur, as one of the promising cathode materials, has benefits such as low toxicity and cost relative to other cathode materials and large natural abundance. This material consists of multiple eight-membered sulfur rings that are held together by van der Waals forces. By using density functional theory, we modeled reactions for Li-S and Ca-S batteries, where sulfur rings are broken forming various Li_{2}S_{x} and CaS_{x} (1 < x < 8) polysulfides. We are specifically interested in calculating the voltage profile, reaction mechanisms, and how the structure of the cathode changes upon charge and discharge. Preliminary work has shed light on the stability of various polysulfide species that form during operation and their relative voltage values. Additionally, some results from the lithium-sulfur battery calculations will be compared with existing literature to demonstrate the accuracy of our modeling. By projecting similar methodology, we also obtained preliminary results for calcium-sulfur as well.
P19. First-principles investigation of Rashba Effect in Two-Dimensional Materials

Authors: Arjyama Bordoloi\textsuperscript{1}, Sobhit Singh\textsuperscript{1,2}

Affiliation: (1)Department of Mechanical Engineering, (2)Materials Science Program, University of Rochester

Abstract: Spintronics, unlike conventional electronics, leverages the spin degree of freedom as a fundamental unit for the storage and transfer of information. The use of spin, rather than charge, enables the design of more energy-efficient and faster non-volatile memory and logic devices. Rashba spin-orbit coupling (RSOC) is one of the most widely used spin-orbit coupling (SOC) effects in designing spintronic devices, particularly using nonmagnetic materials. RSOC primarily originates from the crystal-potential gradient induced by broken structural inversion symmetry in periodic crystals. Hence, unlike other spintronic devices based on giant magnetoresistance and tunneling magnetoresistance, RSOC-based devices do not require any external magnetic field. In this work, we investigate the RSOC effect in various two-dimensional systems (buckled hexagonal and Janus monolayers) using first-principles density-functional theory calculations. Our lattice dynamics and elastic constant calculations ensure the dynamical and mechanical stability of the studied monolayers. Our electronic structure calculations, considering SOC effects, reveal the presence of large RSOC in the studied monolayers. In particular, the W\textsubscript{2}COT\textsubscript{e} monolayer exhibits a substantial Rashba spin splitting near the Fermi level, with a calculated Rashba parameter (aR) of 0.8 eV Å. Our results shed light on some of the interesting puzzles surrounding these materials, unveiling their potential applications in spintronics.
P20. Valleyphotovoltaics: approaching high efficiency solar cells

Authors: Hasan Ahmed\textsuperscript{1,2}, Vincent R. Whiteside\textsuperscript{1}, Mike Santos\textsuperscript{1}, Tetsuya D. Mishima\textsuperscript{1}, Sethulakshmi J. Sudhakara\textsuperscript{1}, Ian R. Sellers\textsuperscript{1,2}

Affiliation: (1) Homer L. Dodge Department of Physics & Astronomy, University of Oklahoma, (2) Department of Electrical Engineering, University at Buffalo

Abstract: We speak about the importance of pursuing next generation solar cells, focusing on the losses associated with the thermalization of charges. Hot carrier cells boast a theoretical maximum efficiency upwards of 60%, significantly more than that suggested by Shockley–Queisser limit. We cover some of the history of the group in working towards this goal in QW systems. We then introduce valleyphotovoltaics, a novel approach whereby the higher density of states in the X and L valley of a device can be used to capture electrons of higher energy, which can curb some of the thermalization losses. We then present how we use photoluminescence to show that this phenomenon is evident in some of our past work and the path forward in designing heterostructures with III-V semiconductors, such as GaAs, that can potentially extract hot electrons, hence the name, hot carrier solar cells. We conclude with some of the hurdles to overcome in exploiting this phenomenon.

Author: Matthew Weil

Affiliation: Ithaca College & NASA SARP

Abstract: Tidal wetlands play a vital role in providing essential ecological services and supporting biodiversity. However, these ecosystems have been adversely impacted by human activities, leading to widespread degradation and loss. In the Chesapeake Bay region, restoration goals aim to reintroduce native vegetation and restore natural hydrological regimes. To assess the effectiveness of tidal wetland restoration, vegetation surveys are essential. Traditional ground-based sampling is time-consuming and provides limited spatial coverage. To overcome these limitations, we leveraged remote sensing techniques to create species-level vegetation classification maps for a restored wetland. We focused on the VCU Rice Rivers Center tidal freshwater wetland, Kimages Creek, in Charles City, Virginia. High-resolution imagery of the restored wetland was obtained using a Wingtra Gen II Unmanned Aerial System (UAS) equipped with the MicaSense RedEdge Panchromatic Multispectral Camera. This UAS dataset served as the foundation for creating species-level vegetation classification maps using a Random Forest machine learning model. The model was trained on ground truth data collected during the UAS image acquisition and incorporated spectral signatures to accurately classify different vegetation species within the wetland. To further enhance the spatial coverage and scalability of our study, we employed a super sampling technique to augment the resolution of Landsat imagery to that of the UAS resolution, allowing us to retain the detailed species-level accuracy achieved through our UAS-based vegetation classification model, now using satellite data. By integrating ground, airborne, and satellite datasets, our study demonstrates the potential of remote sensing techniques, coupled with machine learning models, in monitoring tidal wetland restoration with species-level accuracy.
P22. Raman Spectroscopy study of strain and defects in Chemical Vapor Deposition grown Transition Metal Dichalcogenides

Authors: Rafael N. Gontijo, Samarra L. Grasier, Xintong Ding, Ana Laura Elias Arriaga

Affiliation: Physics Department, Binghamton University

Abstract: Transition metal dichalcogenides (TMDs) are layered materials that present interesting properties in the single layer regime, such as the presence of a direct bandgap. For a large-scale production of TMDs, one method that possesses great potential is the Chemical Vapor Deposition (CVD), which can produce atomically thin films in the mm$^2$ range. However, the films are generally prone to show a large concentration of defects in the form of chalcogen vacancies as well as being subjected to strong strain effects due to the growth procedure, which asks for a way to quickly characterize the grown films for their quality. Raman Spectroscopy is a good way to characterize two-dimensional materials for their quality and defect concentration as well as strain through the observation of deviations in the frequency of the vibrational modes. In this work, we combine Raman and Photoluminescence spectroscopies to characterize strain and defects in CVD grown MoS$_2$, an exemplary TMD. Through the changes in the PL spectrum, we could characterize the strain of over 100 samples by their exciton peak, which is used as a reference for the strain suffered by the sample. By comparing the Raman Data to the PL position, we can indirectly infer the rate of change of the phonons as a function of strain, which can be used to extract the Grüneisen parameter of different phonons. We also show how the intensity of the defect-induced bands can be affected by how strained the crystal is, which directly affects the resonance with the exciton.
P23. Searching for Strong Gravitational Lenses in DESI Spectra

Authors: Delaney Cummins\textsuperscript{1}, Segev BenZvi\textsuperscript{1}, Xinyi Chen\textsuperscript{2}

Affiliation: (1)Department of Physics and Astronomy, University of Rochester, (2)Department of Astronomy, Yale University

Abstract: Strong gravitational lensing systems are typically observed in imaging surveys via rings, multiple images, or other visual effects affecting the source galaxy. However, we expect to see 5 to 10 times more strong lensing systems with Einstein radii smaller than the resolution of most imaging surveys. These systems may be found using spectroscopy, and their detection would dramatically increase the number of known lensing systems, improving our chances to perform time-delay cosmography and other cosmologically significant studies. We train a vision transformer (ViT) and a convolutional neural network (CNN) to find strong lensing systems in DESI spectra. The ViT and the CNN displayed similar levels of performance on this problem, classifying lenses and non-lenses with >85% accuracy.
P24. Detecting Gravitational Waves Using Pulsars

Authors: Sophia Sosa Fiscella, Dr. Michael Lam, NANOGrav Collaboration

Affiliation: School of Physics & Astronomy, Rochester Institute of Technology

Abstract: The potential of pulsar radioastronomy was proven this year with the first evidence for a gravitational wave background in the dataset of the North American Nanohertz Observatory for Gravitational Waves (NANOGrav). In this work we present a proof-of-concept of a method for improving the timing precision currently achieved with NANOGrav’s 12.5-years dataset. We selected a 12-seconds long observation of PSR J2145−0750 at the Green Bank Telescope, we classified its single pulses into clusters using the K-means method of vector quantization, and then we weight-averaged the cluster times of arrival based on their error. This method could potentially help improve the timing precision for certain datasets of bright pulsars in NANOGrav’s dataset.
P25. Elastic and Electronic Characterization of KNb$_3$Sb$_5$ and KTa$_3$Sb$_5$ Kagome Metals: An Ab-initio Study

Authors: Chao-en “Aaron” Chuang, Yifan Wei, Sobhit Singh

Affiliation: (1)Department of Mechanical Engineering and (2)Materials Science Program, University of Rochester

Abstract: Since the discovery of the first kagome material, FeSn, in 2018, hexagonal networks of triangles in 2D atomic lattices have gained prominence as a captivating class of compounds exhibiting unique quantum phenomena such as frustrated magnetism, superconductivity, charge-density wave ordering, and topological flat bands. These materials have the potential to revolutionize next-generation technology, especially spintronics. Building on the discovery of the kagome family, MV$_3$Sb$_5$ (M=K, Rb, Cs), where the kagome network is transitioned from V to Nb and Ta, this research focuses on the investigation of the novel compounds KNb$_3$Sb$_5$ and KTa$_3$Sb$_5$, with a particular emphasis on their electronic, elastic, and mechanical properties. We conducted first-principles density functional theory calculations to determine the optimized lattice parameters, elastic moduli, and electronic bandstructure of the studied compounds. Our calculations reveal that KNb$_3$Sb$_5$ and KTa$_3$Sb$_5$ exhibit ductile metallic behavior, characterized by multiple topologically nontrivial electronic band crossings near the Fermi level. The computed elastic moduli of these two compounds yield an average bulk modulus of 33.9 GPa, shear modulus of 8.9 GPa, and Young's modulus of 22.5 GPa. Further, we discuss the role of spin-orbit coupling on the electronic and elastic properties of the studied metals.
P26. Scalable Synthesis of Monolayer WSe$_2$ and MoSe$_2$ via Aqueous Precursor CVD for Optoelectronic Applications

Authors: Nilupa Gunarathna, Rafael Nunez Gontijo, Ana Laura Elias

Affiliation: Department of Physics (Applied Physics & Astronomy), SUNY Binghamton

Abstract: This study addresses the challenge of synthesizing two-dimensional (2D) transition metal dichalcogenides (TMDs) in a scalable manner. The TMDs focused on are Molybdenum Diselenide (MoSe$_2$) and Tungsten Diselenide (WSe$_2$), which have potential applications in optoelectronic devices such as photovoltaics. MoSe$_2$ and WSe$_2$ are group VIB TMDs with layered crystal structures and unique excitonic features that become apparent with decreased layer numbers. In the monolayer regime, both MoSe$_2$ and WSe$_2$ transition from being indirect to direct bandgap semiconductors, which gives rise to their direct bandgap and strong excitonic transitions. Furthermore, monolayers of MoSe$_2$ and WSe$_2$ exhibit efficient light absorption, large carrier mobilities, and tunable energy band structures. In this study, we present a novel Chemical Vapor Deposition (CVD) methodology for large area monolayer MoSe$_2$ and WSe$_2$ fabrication. This process involves spin-coating an aqueous phase precursor solution onto SiO$_2$ wafers, followed by high-temperature annealing and selenization to yield uniform monolayer growth. We achieved high-quality, millimeter-scale MoSe$_2$ and WSe$_2$ monolayers through optimization of key parameters such as growth temperature, precursor concentration, and metal precursor/surfactant ratio. The synthesized MoSe$_2$ and WSe$_2$ exhibit excellent optical properties, as confirmed by Raman spectroscopy and photoluminescence measurements. Specifically, monolayer samples exhibit strong emission peaks at approximately 1.58 eV for MoSe$_2$ and 1.65 eV for WSe$_2$, which are attributable to the neutral exciton and indicative of a transition from indirect to direct bandgap.
**P27. Exploration of Superconducting Properties of Conventional Superconductors via Machine Learning Methods**

**Authors:** Benjamin Smoker, Yasantha Pasindu Hetti Kankanamalage, Sachith Dissanayake, and Sobhit Singh

**Affiliation:** (1)Department of Mechanical Engineering, (2)Materials Science Program, University of Rochester

**Abstract:** The discovery of superconductors, characterized by their zero electrical resistance and magnetic field expulsion, has led to transformative technologies like hypertrains. However, utilizing superconductors to their full potential is challenging due to their requirement for extremely low temperatures and, in some cases, high pressures. This has spurred efforts to discover superconducting materials that can function under ambient conditions. Machine learning (ML) has been a valuable tool in this quest, but the need for extensive datasets has limited its applicability, with errors of up to 50% in existing models that were trained on a theoretical database of superconducting materials. This study addresses this issue by incorporating experimental data to improve the predicted power of ML models. Through a two-step process involving transfer learning, we first train our ML model on the JARVIS dataset, a theoretical database, and then apply it to experimental superconductors using their critical temperature and crystallographic information. This approach enables our model to establish correlations between crystallographic data and superconducting properties, with additional improvements made by integrating experimental data.
**P28.** Achieving a Linear Synaptic Update in 2D Crystal Gated Field Effect Transistors for Applications in Artificial Neural Networks

Authors: Cori Sutton, Nithil Harris Manimaran, Shubham Awate, Ke Xu


Abstract: In order to overcome the Von Neumann bottleneck and increase the power efficiency of modern computation, neuromorphic computing has emerged as a potential solution which allows for parallel computing, adaptive learning, and long-term potentiation for use in neural networks. Electric double layer (EDL) transistors use ions to induce a high charge carrier density inside the channel, and both long and short term ionic response closely resembles a biological synapse. EDLTs based on 2D crystal allow for low power operation, making it a promising candidate for use in artificial neural networks. In order for EDLs to be viable for this application a linear synaptic response is highly required (a proportional weight update in response to a voltage input), however this has proven to be challenging with a constant input voltage for a given frequency. This study examines the reasons why we see a non-linear weight update, caused by the induced electric field between ions resulting in an exponential decay between input pulses, related to the concentration of the EDLs. This leads to an increasing rate of weight decay, which eventually stagnates the output signal resulting in no weight update over concentric pulses. This behavior was examined uses Finite Element Modeling within COMSOL using the modified Nernst-Poisson-Planck equations. 10 pulses were given as input at 100Hz, and as expected the EDL concentration saturated within these 10 pulses at less than half of the maximum concentration possible with the same steady voltage. Next we were able to show that a linear EDL concentration was possible through a varying magnitude voltage (i.e nonlinear input). The challenge with this approach comes with the non-linear dissipation between pulses, making it necessary to predict the dissipation and required voltage. Based on the change in EDL concentration over time (dc/dt) we were able to create an empirical relationship between (dc/dt), concentration and input voltage which we were then able to couple with the COMSOL model to predict the necessary inputs in a single computation. For the 100Hz trial over 10 pulses a linear weight update with R² of 0.996 was achieved with a 13% increase is final EDL concentration with inputs ranging between 0.25-3V (within the electro-chemical window of PEO:LiClO₄) and still has potential to continue to increase, which was not possible with a constant input magnitude. These preliminary findings show possibilities for extending this behavior for use in artificial synapses and EDL based synaptic networks. Moving forward the group is focused on experimentally verifying the model parallel plate capacitor geometry and graphene-based EDL transistors.
Critical Examination of Cross Quantum Capacitance on Electric Double Layer Gated 2D Field Effect Transistors

Authors: Jacob Eisensmith, Ke Xu

Abstract: 2D semiconductor materials have been a focus of study for applications in next generation electronic devices due to their unique properties including high electrical and thermal conductivity. These properties along with their unique band structures enable novel physics and applications including semiconducting to metallic (and even to superconducting) phase transitions. To achieve such transitions, an ultrahigh local electric field and capacitance is required. Electric double layer (EDL) gating is a technique that uses ions in an electrolyte to control charge transport in an electronic material by field-effect, and has been demonstrated to induce high local electric fields (>1V/nm) and capacitance density (>1uF/cm2) on a variety of 2D crystals [1]. In addition to geometric capacitance, quantum capacitance, related to the chemical potential of charge carriers in the semiconducting material, has acted as a parasitic capacitance that limits the total capacitance and carrier concentration. Recent investigations have revealed that quantum capacitance alone does not fully account for the loss of capacitance in experimental measurements. An additional cross quantum capacitance (CQC) has been proposed [2, 3]. The CQC considers coulombic interactions between charges on the same “plate” of the capacitor and those of the opposing plate. Such interactions become significant only when the distance between the two plates of capacitor is sufficiently small, which is the case for EDL formed between ion conductor and monolayer 2D crystal. While some experimental studies have attributed the lower measured conductivity to CQC, none of them analyzed the experimental data based on CQC equations to prove or quantify the impact of CQC [2, 3]. In this study we conducted a critical examination of the theory of CQC [4], and our findings suggest that only under specific conditions would CQC decrease the total capacitance. We evaluate the conditions in which it may present itself and whether/how these conditions are physically realizable, these findings may help suggest device parameters to maximize the total achievable capacitance in EDL gated 2D crystal FETs.
P30. Switching Behavior in NbO2-Based Memristive Devices

Authors: Matthew C. Sullivan, Uday Lamba

Affiliation: Ithaca College

Abstract: To meet the growing needs of computing, we depend on the fabrication of increasingly miniaturized transistors and the denser integration onto semiconductor chips. This trend would not continue as we approach fundamental physical limits due to the extremely small feature size. Studies suggest computational energy needs will exceed global energy production by 2040. Modern computing devices are based on the Von Neumann architecture, and a significant amount of energy is spent moving data back and forth between memory and the processor. Memristor-based brain-inspired neuromorphic architecture can help with this fundamental challenge. The new architecture can do in-memory computations eliminating the energy spent on data transfer. Memristors can dynamically change their resistance in response to electrical stimuli making them perfect for mimicking the switching behavior of neurons. We fabricated niobium dioxide (NbO2) based memristive devices and examined their characteristics. These devices showed excellent switching behavior making them highly favorable candidates for future research. We are currently exploring techniques to optimize and further improve the switching behavior of the memristors. Our work contributes to advancing the understanding of memristive devices for applications such as artificial intelligence, non-volatile memory, and neuromorphic computing.
**P31. First-Principles Investigation of Elastic and Mechanical Properties in Kagome Metals CsM₃Te₅ (M = Ti, Hf, Zr)**

**Authors:** Yifan Wei, Chao-En “Aaron” Chuang, Sobhit Singh

**Affiliation:** (1)Department of Mechanical Engineering, (2)Materials Science Program, University of Rochester

**Abstract:** Kagome metals are a unique class of quantum materials characterized by their distinct atomic lattice arrangement, featuring interlocking triangles and expansive hexagonal voids. These lattice structures impart exotic properties, including superconductivity, topology, and magnetism, among others. Among these materials, CsM₃Te₅ (M = Ti, Zr, Hf) has been previously confirmed to exhibit superconductivity and nontrivial topological properties. However, the predominant focus of research has centered on their superconducting characteristics, resulting in a lack of attention to their elastic and mechanical properties. This study employs first-principles density functional theory calculations to predict the elastic and mechanical properties of CsM₃Te₅ (M = Ti, Zr, Hf). Our calculations reveal that the studied compounds - CsTi₃Te₅, CsZr₃Te₅, and CsHf₃Te₅ - are ductile metals with elastic properties akin to tin (Sn), with average elastic constants, including a bulk modulus of 26.9 GPa, a shear modulus of 10.1 GPa, and Young's modulus of 26.0 GPa. Notably, we observe a decreasing trend in all elastic constants as the atomic number increases from Ti to Hf, with CsTi₃Te₅ displaying considerably larger elastic constants in comparison to the other studied compounds, underscoring its importance for further research into their fundamental behaviors and other mechanical properties.
P32. Realizing Gate-All-Around Vertical Nanowire Field-Effect Transistors Based on Van Der Waals Epitaxial InAs-on-2D Heterostructures

Authors: John Wyatt Morrell1,2, Alireza Abrard3,4, Nithil Harris Manimaran4, Parsian K. Mohseni2,3,4,5, Ke Xu1,2,4


Abstract: III-V semiconductors show promise as channel materials in next generation nanoelectronics. Among III-V materials, InAs stands out as a potential replacement for n-type channel material in complimentary metal-oxide-semiconductor (CMOS) based devices. Compared with silicon, InAs offers 30 times the electron mobility and a higher ON current, and when grown as a 1D InAs nanowire (NW), this mobility is further enhanced compared to thin-film and bulk InAs. As such, NW FETs were developed to harness the potential of III-V materials, where a gate-all-around (GAA) geometry offers better electrostatic gating of NWs but proves to be a much more difficult fabrication process, especially with vertical NWs. In order to solve this issue, electric double layer (EDL) gating can be used. EDL gating is a method which uses an electric field to control mobile ions within an electrolyte to create strong local electric fields. Due to the accumulation of ions in the electrolyte ~1 nm from the channel, fields on the order of 10 MV/cm can be achieved, allowing for high carrier density in semiconducting materials (including 2D and III-V materials). Additionally, the strength of EDL gating is weakly dependent on gate to channel distance, which allows for flexibility in device geometry without sacrificing carrier density. EDL gating can support otherwise difficult to fabricate geometries such as vertical GAA NW FETs. In this study, we will investigate the challenges that come with fabricating these novel devices, as well as electrical characterization. The device geometry consists of dense vertical InAs NW fields epitaxially grown on graphene, with solid electrolyte permeating between NWs, topped with a metal electrode contacting the top of the NWs. Characterization of the fabrication process and its impact on the integrity of the NW will be performed on via AFM, RAMAN, and SEM analysis.
P33. Transition Metals for Silicon-based Anode Materials

Authors: Alhamdu Nuhu Bage,1 Dr. Howard Tu2

Affiliation: (1)Department of Chemical Engineering, (2)Department of Mechanical Engineering, Rochester Institute of Technology

Abstract: The primary factors leading to the utilization of transition metals (TMs) in the production of silicon-based lithium-ion batteries (LIBs) composite anodes are their robustness, electrical conductivity, flexibility, resistance to lithium reactions, and adjustability. TMs play a significant role in enhancing the overall electrochemical efficiency of LIB electrodes by counteracting the undesired expansion of silicon. The impact of various elemental transition metals, including copper (Cu), titanium (Ti), nickel (Ni), and iron (Fe), on the electrochemical performance of silicon-based composites was assessed, and the phases formed during the milling process were connected to the behavior of the composites they are found in. Nickel, copper, titanium and iron alleviated mechanical stresses, improved stability, electrical conductivity and resistance to deformation respectively and alongside other metals in each composite formulation provided a robust matric capable of buffering silicon expansion. The internal and microstructural properties of silicon need to be designed in a distinct fashion in order to overcome its inherent limitation in electrochemical applications. In this work, composites of TiFeSiC, employing micro, nano, and porous silicon, exhibited reversible capacities of 990.45 mAh.g\(^{-1}\), 1137.69 mAh/g, and 1045.43 mAh/g at C/10. The findings from electrochemical characterization indicate that the porous structure within the composite anode material, created through acid etching, mitigated silicon expansion during the lithiation/delithiation process. The void spaces formed within the porous silicon’s inner structure, along with the presence of carbon, enhanced electronic conductivity among silicon particles while reducing the overall diffusion distance of Li+. 
P34. Modeling Current Flow Through Copper with Surface Substituted Intermetallic Barrier Layers

Authors: Matthew Jankowski, Kevin Batzinger, Manuel Smeu

Affiliation: Department of Physics, SUNY Binghamton

Abstract: With the continuous shrinking of integrated circuits comes the likewise size reduction of their interconnects. This comes at the cost of increased resistivity of the interconnects, being exacerbated by surface roughness which is required for adhesion to circuit components. The size of these interconnects, being on the order of a few nanometers, warrants consideration of electronic scattering effects to determine their transport behavior. We employ a first-principles approach using density functional theory (DFT) in conjunction with the Keldysh non-equilibrium Green’s functions (NEGF) formalism to determine the electronic structure of nanoscale Cu interconnects with roughened intermetallic barriers under a bias voltage. Tangible properties such as conductance are recovered with NEGF-DFT. We hypothesize that introducing a barrier layer may mitigate electronic scattering at the roughened surface and recover some of the conductance that is lost when said roughness is introduced in a pure Cu interconnect. In particular, we probe barrier layers composed of Mn, Ni, Zn, Ag, Sn, and Cu3Sn with five distinct roughness configurations, where half of the top barrier layer atoms have been randomly removed. We also investigate the effects of a non-ideal interface by intermixing barrier layer atoms below the roughened surface, creating an “interphase” between the barrier and the Cu film.
**P35. Progress on Substrate Reuse Using Sonic Lift-Off for GaAs-Based Photovoltaics**

**Authors:** Andrew Sindermann, Elijah Sacchitella; presented by Brandon Bogner

**Affiliation:** Rochester Institute of Technology

**Abstract:** Sonic lift-off is able to reduce average surface facet amplitude without degrading bulk material quality and is thus a promising technology for enabling repeated substrate reuse with GaAs-based photovoltaics. 1-sun AM1.5G illuminated current density-voltage data and spectral response data from four devices at different stages of the spalling process have been presented. Devices grown on a commercial substrate and then acoustically-spalled as well as devices grown on a previously acoustically-spalled substrate with minimal surface treatment did not show degradation in device performance compared to the control grown on a commercial substrate, which was 17% efficient without anti-reflection coatings. Devices grown on a previously acoustically-spalled substrate and then spalled exhibited degradation in both short-circuit current density and open circuit voltage for a final 8% efficiency, indicating further process improvements are necessary to realize efficient substrate reuse.