Welcome to Materials Day 2017

Welcome to Materials Day at Penn State, sponsored by the Materials Research Institute. MRI is composed of 250-plus materials-related faculty and their research groups at University Park and Commonwealth campuses. MRI operates four open user facilities for modeling and synthesis, nano- and micro-fabrication, materials characterization, and 2D crystal synthesis. The latter, the Two-Dimensional Crystal Consortium-Materials Innovation Platform (2DCC-MIP), is a new national user facility supported by the National Science Foundation (DMR-1539916).

The goals of the 2DCC-MIP are to discover novel 2D materials for next generation electronics, engage industry, government, and academia through an external user program, and train the next generation of scientists in two-dimensional and layered materials. In addition to engaging directly with the MRI’s other facilities, the 2DCC-MIP has state-of-the-art instrumentation and expertise distributed in three user facilities: Thin Films Synthesis and In Situ Characterization, Bulk Crystal Growth, and Theory and Simulation. Visit their website for a complete overview: mri.psu.edu/mip.

We are witnessing the convergence of the life sciences and the physical sciences, a frontier epitomized by the two interdisciplinary institutes housed within the Millennium Science Complex. Of particular note on this theme is the installation of the University’s first cryogenic transmission electron microscope, in the basement level of the MSC. This instrument is being set up to accommodate both life sciences and materials science researchers, with expertise drawn from both the Huck Institutes of the Life Sciences and MRI, as well as the Penn State College of Medicine.

And in the MRI Nanofab, the world’s highest-resolution 3D printer is now online. With sub-micrometer resolution, the Nanoscribe Photonic printer can print feature sizes down to 200 nm.

Hot Topics
This year’s program features interactive breakout sessions on eight “hot topics” in the materials community. The format of each session is designed for maximum audience participation. Panelists will provide expertise from industry, government, and academic perspectives. Each session chair will conclude their breakout with a high-level summary. Enjoy the conversation, the keynote address and reception, and the interactive poster session.
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Agenda

Tuesday, October 17
All agenda items for Tuesday will be in the Nittany Lion Inn

10:00 a.m.  Registration

11:00 a.m. – 2:00 p.m.  Poster Session
Posters will be presented by many of the Materials Research Institute faculty groups and provide an interactive opportunity to get a snapshot of the breadth of research in materials at Penn State.

11:00 a.m. - 2:00 p.m.  Live SMS polling to vote for your favorite poster

12:30 p.m. – 1:30 p.m.  Lunch

2:30 p.m. – 4:30 p.m.  Breakout Sessions

“Functional Materials by Design” - Ismaila Dabo
Virtual experiments from atoms to systems [Boardroom 2]

“Humanitarian Materials” - Esther Obonyo
Materials at a human scale [Penn State Room]

“Advanced and Sustainable Manufacturing” - Douglas Wolfe
New ways of making [Alumni Lounge]

“2D Materials” - Joshua Robinson
Building materials one layer at a time [Boardroom 1]

5:00 p.m. – 7:45 p.m.  Keynote Reception

“Aerospace Materials for Extreme Environments”
Ali Sayir, Air Force Research Program Manager
Introducing the Keynote:
Clive Randall, MRI director, with the State of the Materials Research Institute. Top voted posters and tabletops displays on site.
Agenda (continued)

Wednesday, October 18
All agenda items for Wednesday will be in the Millennium Science Complex

8:00 a.m. Registration
Coffee and pastries will be provided [3rd Floor Commons]

9:00 a.m. – 11:00 a.m. Breakout Sessions

“Advanced Fibers and Smart Textiles” - Melik Demirel
Recreating an industry by adding value and sustainability [N-203A/B]

"Redesigning Catalysts at the Nanoscale” - Michael Janik
Reaction mechanism in nanoscale systems [N-201]

"Materials for Health” - Jian Yang
The road from biomaterial science to medical devices and patient care [N-050]

"Electronic and Photonics on the Horizon” - Chris Giebink
What are we building in the lab today that will matter tomorrow? [N-308A/B]

11:30 a.m. – 1:00 p.m. Breakout Sessions Chairs’ Report-Outs
Lunch will be provided [3rd Floor Commons]

1:00 p.m. – 3:00 p.m. Industry Tours:
Millennium Science Complex,
CIMP-3D, or
Stiedle Building (newly renovated and reopened July 2016)
Ali Sayir  
Air Force Office of Scientific Research and NASA Liaison

Aerospace Materials for Extreme Environments

Bio
Dr. Sayir is currently the Program Manager of Aerospace Materials for Extreme Environments at AFOSR. Dr. Sayir received his Ph. D. in 1990 in Materials Science and Engineering from Case Western Reserve University and held a Diplom Ingenieur Degree from the Technical University of Clausthal, Germany. Dr. Sayir joined NASA Lewis Research Center (now Glenn) in 1990 as a National Research Council awardee. Upon joining NASA Glenn, he began a career of eutectic solidification and basic research in polyphase microstructures. He has made contributions in the development and use of advanced high strength, single crystal fibers for high temperature applications, piezo-ceramics with higher temperature capability for actuation devices, and thermoelectric materials and space power applications.

Dr. Sayir has served on national and international committees, and has over 50 invited presentations for the American Ceramic Society, American Physical Society, European Ceramic Society, Electrochemical Society and Materials Research Society. He organized five International Workshops and co-organized 11 symposiums with American Ceramic Society and published over 120 peer-reviewed journal publications. He has been a Fellow of the American Ceramic Society since 2010. He received the Medal for Public Service Award (2003), R & D 100 Award for Laser Fiber Growth (1993), NASA Inventions Board Awards (2009, 2008, 2007), and received numerous recognitions from Industry and government laboratories.

As Point of Contact for Materials and Structures of NASA Hypersonic program, he coordinated materials and structures projects between NASA centers, Department of Defense, Industry and Academia. Since 2008 he has held a Research Associate Professor faculty appointment at Case Western Reserve University in the Department of Materials Science of Engineering and since 2005 has held an adjunct faculty appointment in the Department of Mechanical Engineering at the University of Akron.

Abstract
Transformative breakthroughs most of the time do not originate from the investigations of materials in the equilibrium state but in contrary at the margins of stability, in a regime at the limit or outside of the textbook knowledge within the discipline. In this context, this presentation will embrace materials and processing science approaches that are far from the thermodynamic equilibrium domain; i.e., directionally solidified eutectic structures, highly doped piezoelectric and thermoelectric materials, and other oxide materials with cage structures for electron emission. The intent is to elucidate the complex interplay between phase transitions for electronic/magnetic phase separation and untangle the interdependence between structural and electronic effects. I will also discuss what I consider to be promising research concentration areas within ceramics research for the aerospace materials for extreme environments portfolio of Air Force Office of Scientific Re3search(AFOSR), including the focused development of a ceramics processing science laboratory for ceramic matrix composites, the development of materials for use in the hypersonic regime.
## Reception Tabletops

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<td>Mark Leiby</td>
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<td>Heidi Siwik</td>
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Breakout Session:

Functional Materials by Design
Virtual Experiments from Atoms to Systems  

Tuesday, October 17 | 2:30 p.m. – 4:30 p.m.

Abstract

Progress in synthetic chemistry and layer-by-layer assembly has opened up the possibility to design materials that respond in a prescribed way to external constraints, making it feasible to achieve desired functionalities by precise control of their structure and composition. These functional materials have profoundly transformed the technological landscape, pushing back the frontiers of device performance and miniaturization with applications in, e.g., energy storage and conversion and optoelectronic nanotechnologies. Considering the central role played by functional materials in technological innovations, there is a critical need across academia, industry, and national laboratories to develop the fundamental knowledge, technical expertise, and infrastructural capabilities for supporting the discovery, development, and deployment of these materials. This breakout session will bring together researchers from academia and industry to explain how recent advances in computational modeling are being leveraged to solve the inverse design problem of identifying novel materials with targeted functional responses. The remaining challenges facing the computational design of functional materials will also be discussed.

Panelists


- Dr. Boris Kozinsky – Principal Scientist, Robert Bosch Research and Technology Center
- Dr. Michael Makowski – Technical Platform Manager, PPG Industries
- Dr. Adama Tandia – Research Associate, Corning Inc.
- Prof. John Keith – assistant professor of chemical and petroleum engineering, University of Pittsburgh
- Prof. Michael Janik – associate professor of chemical engineering, The Pennsylvania State University
- Prof. Adri van Duin – professor of mechanical and nuclear engineering, The Pennsylvania State University
Breakout Session:

Humanitarian Materials
Materials at the Human Scale  

Tuesday, October 17 | 2:30 p.m. – 4:30 p.m.

Abstract

The innovative design and synthesis of transformational building materials can significantly advance efforts directed at catalyzing economic development at the regional scale through narrowing the global infrastructure gap. Building materials account for one-third of the total cost of construction. This session will focus on identifying specific ways through which the transformational use of humanitarian materials would result in transformative impact for the society through reducing construction costs. It will also enhance the optimal use of scarce materials in building systems, which over time function in an eco-efficient manner. There is a broad scope for addressing these needs through novel use of building materials. These range from the incremental improvements to traditional materials and existing characteristics, to the synthesis of new material combinations with additional multifunctional characteristics, to radical innovation in materials with entirely new functionalities. Clearly, this vast opportunity for innovation has attracted a lot of attention from researchers across the globe. This notwithstanding, the existing market-ready materials cannot be deployed easily in a low-income context at the scale that would result in transformational impact for economic development, environmental sustainable, and social prosperity. Leaping successfully over what has become the “valley of death” for many of the non-conventional building materials requires a living lab approach, which allows the key decision makers to incorporate input and feedback from all the stakeholders along the value chain in a timely manner. The panel discussions in this session leverage a new initiative directed at revitalizing New Kensington, PA, into a vibrant community that supports economic growth and sustainable development through entrepreneurism and innovation. A consortium led by The Pennsylvania State University (New Kensington and University Park) and Arconic Technology Center is championing the initiative. The outcomes of this initiative can be adapted for deployment in other low-income communities such as other Rust Belt areas and across the globe in emerging economies such as Sub-Saharan Africa.

Panelists

Moderator: Esther Obonyo – associate professor of architectural engineering and engineering design, The Pennsylvania State University

- Chancellor Kevin Snider – The Pennsylvania State University, New Kensington
- Mr. Stephen B. Leonard – Senior Innovation Lead, Arconic Technology Center
- Ms. Sarah Snider – Volunteer Chair, New Kensington Corridor of Innovation
- Prof. Clive Randall – Director, Materials Research Institute, professor of materials science and engineering
Breakout Session:

Advanced and Sustainable Materials
New Ways of Making (Additive Manufacturing)

Tuesday, October 17 | 2:30 p.m. – 4:30 p.m.

Abstract

Additive manufacturing (AM) technologies have opened a design space that offer the potential to revolutionize how some components are manufactured in that new and novel components and systems can now be fabricated which previously could not due to the complexity of the manufacturing operations. These manufacturing innovations are pushing performance capabilities to new heights in both industrial and defense sectors. There are numerous benefits associated with additive manufacturing for polymers, metals, ceramics, and composites (PMC, MMC, CMC) ranging from commercial products to prototypes but there are still some challenges. This break out session will discuss the various successes with regards to commercial and government implementation and interest as well as future challenges and research opportunities in powder design characteristics/specifications, printing components with the correct geometry and dimensions, part qualification, economic advantages, component size, resolution, etc. that will further develop this technology. The Pennsylvania State University is home to the Center for Innovative Materials Processing through Direct Digital Deposition (CIMP-3D) which is a world-class resource for advancing and deploying additive manufacturing (AM) technology for critical applications. With a broad mission to advance and deploy AM technology of metallic and advanced material systems to industry, technical assistance to industry through selection, demonstration, validation training, education and dissemination of information.

Panelists


- Dr. Richard Martukanitz — Co-Director CIMP-3D, Applied Research Laboratory, The Pennsylvania State University
- Prof. Allison Beese — assistant professor of materials science and engineering, The Pennsylvania State University
- Dr. William Frazier — Chief Scientist, Air Vehicle Engineering, Naval Air Systems Command (NAVAIR)
- Dr. David Furrer, Senior Fellow and Director of Manufacturing Technologies, Pratt and Whitney Corporation
- Dr. James Sears, Principal Engineer, Carpenter Technologies Corporation
Breakout Session:

2D Materials
Building Materials One Layer at a Time  

Abstract

Two-dimensional materials have been touted as next-generation materials for electronics, photonics, coatings, and composites for more than a decade now. Key to the success of 2D materials will be our ability to conduct leading international and multidisciplinary research on 2D layered materials aiming at finding new phenomena and applications that could be transformed into high-impact products. The Pennsylvania State University has three major centers focused on 2D materials that offer a unique, vertically integrated opportunity to span fundamental science to application, with extremely valuable components including state-of-the-art infrastructure and research environment. During this breakout session, we will discuss the spectrum of opportunities 2D materials may offer, and how these opportunities may be realized into tomorrow’s technology.

Panelists

Moderator: Josh Robinson – associate professor of materials science and engineering, The Pennsylvania State University

- Dr. Robert Lee – Surfaces Research Thin Films and Surfaces Science & Technology Manager, Corning Inc.
- Dr. Nicholas Glavin – Materials Scientist, Air Force Research Lab
- Mr. Richard Clark – Senior Technical Specialist, Morgan Advanced Materials
- Prof. Nitin Samarth – professor of physics, The Pennsylvania State University
Breakout Session:

Advanced Fibers and Smart Textiles
Recreating an Industry by Adding Value and Sustainability

Wednesday, October 18 | 9:00 a.m. – 11:00 a.m.

Abstract

Recent advances in the nanotechnology of fibers and textiles, combined with parallel improvements in biotechnology and synthetic biology, have demonstrated that more complex materials with properties engineered precisely to optimize performance can be achieved. These technologies will transition to industrial applications in textile through guidance of the fundamental materials science and successful development of synthesis, integration, and evaluation of novel fibers. The themes that form the core discussion of this breakout session include: (i) Develop revolutionary techniques for synthesis of programmable fibers, (ii) Develop smart fibers using self-assembly of layered materials and polymers, (iii) Develop novel chemical and molecular doping methods to tailor smart fibers for optical and electronic applications, and (iv) Develop novel characterization techniques across multiple length scales to correlate the process/property relationship of the fibers and textiles. This breakout session brings together a group of leading academic, industrial, and government scientists to discuss future opportunities in designing advanced and smart fibers for added value and sustainable textiles applications.

Panelists

**Moderator:** Melik Demirel – *professor of engineering science and mechanics, The Pennsylvania State University*

- Dr. Natalie Pomerantz – *Research Chemical Engineer, US Army Natick Soldier Center*
- Dr. Andy Liu – *Fashion Institute of Technology*
- Dr. Barbara Trippeer – *Fashion Institute of Technology*
- Ms. Stephanie Rogers – *Director, Advanced Product Development, Apex Mills Corp.*
- Prof. Felecia Davis – *assistant professor of architecture, The Pennsylvania State University*
Breakout Session:

Redesigning Catalysts at the Nanoscale
Reaction Mechanism in Nanoscale Systems  

Wednesday, October 18 | 9:00 a.m. – 11:00 a.m.

Abstract

Catalysis contributes to greater than 35% of the global GDP or approximately 3.5 trillion dollars in primary areas such as energy (fuel) production, chemicals (materials) production, and foodstuffs. Although the impact of catalysis on our everyday lives and the global economy is immense, the materials we call catalysts are far from perfect. Perfection in a catalytic material is a pursuit at many length scales, but the nanoscale represents the ultimate level at which the interaction between catalysts and feedstocks that are subsequently converted into fuels and chemicals occurs. However, the nanoscale features of catalyst can’t be controlled or tuned as needed leading to inefficiencies in current catalytic materials. To be able to reduce catalytic inefficiencies (i.e., slow production rates, selectivity to undesired products), control of the nanoscale catalyst architecture is imperative. Control at this scale enables catalyst design. Advances in experimental and computational methods and their synergy have enabled catalyst design to become reality. This breakout session brings together a group of leading academic, industrial, and government scientists to discuss future opportunities in catalyst design and the sectors most likely impacted by improved catalytic materials.

Panelists

Moderator: Michael J. Janik – associate professor of chemical engineering, The Pennsylvania State University

- Dr. Michael Reynolds – Regional Discipline Lead - Production Chemistry, Shell Exploration and Production Company
- Dr. Victor Sussman – Core R&D Inorganic Materials & Heterogeneous Catalysis, Dow Chemical
- Prof. Rob Rioux – professor of chemical engineering, The Pennsylvania State University
- Prof. Tom Mallouk – professor of chemistry, materials science, and physics The Pennsylvania State University
Breakout Session:

Materials for Health
The Road from Biomaterial Science to Medical Devices and Patient Care

Wednesday, October 18 | 9:00 a.m. – 11:00 a.m.

Abstract

Undoubtedly, advances in biomaterial science research will bring tremendous opportunities for the innovation of medical devices to address unmet clinical problems. This breakout session brings together a group of outstanding Penn State Biomaterial scientists and surgeons with entrepreneurial experience and leaders in medical device industry to lead the discussion on the opportunities and challenges in biomaterial innovation, technology translation, Startups, FDA regulations, and patient care.

Panelists

Moderator: Jian Yang – professor of biomedical engineering, The Pennsylvania State University

- Prof. Jim Adair – professor of materials science and engineering, biomedical engineering, and pharmacology, The Pennsylvania State University
- Prof. Dan Hayes – associate professor of biomedical engineering, The Pennsylvania State University
- Mr. Donald McCandless – Director, Business Development, Ben Franklin Transformation Services
- Mr. James Malayter – Managing Partner, Acuitive Technologies, Inc.
- Elias Rizk, M.D. – assistant professor of neurosurgery, The Pennsylvania State University College of Medicine and Milton S. Hershey Medical Center
- Mr. Barry Fell – President, SIG Medical Corp.
Breakout Session:

Electronics and Photonics on the Horizon
What We are Building in the Lab Today that Will Matter Tomorrow

Wednesday, October 18 | 9:00 a.m. – 11:00 a.m.

Abstract

The world of electronics is changing. At small scales, we are nearing the end of Moore's law for computing, and light is increasingly replacing copper for signal transmission at the board level today and chip level tomorrow. At large scales, new materials and fabrication approaches are driving a range of opportunities, from flexible displays to photovoltaic windows, biosensors, and implantable devices with exciting potential for human health. Based on input from leaders in industry, government, and academia, this breakout session will explore some of the emerging photonic and electronic devices that will change the way we process and interact with information, use and conserve energy, and improve our health within the next decade.

Panelists

**Moderator:** Chris Giebink – assistant professor of electrical engineering, The Pennsylvania State University

- Dr. Pete Trefonas – Corporate Fellow in Electronic Materials, Dow Chemical Company
- Dr. Mike Haney – Program Manager, ARPA-E
- Prof. Jon-Paul Maria – professor of materials science and engineering, The Pennsylvania State University
- Prof. Tom Jackson – professor of electrical engineering, The Pennsylvania State University
- Prof. Enrique Gomez – associate professor of chemical engineering, The Pennsylvania State University
About the Industry Tours

Visitors to Materials Day from off campus had the opportunity to sign up for one of the tours described below. We also welcome all attendees to take a moment to view the first five posters in our ongoing Materials at Penn State Historical Poster Project.

Millennium Science Complex
Opened in 2011, the Millennium Science Complex is the largest research building on campus at just under 300,000 sq ft. User facilities include the basement-level Materials Characterization Laboratory, Nanofabrication Facility and Two-Dimensional Crystal Consortium labs on the first floor, and numerous shared labs throughout the North wing.

The Steidle Building
This beautifully renovated building retains the iconic front exterior of the original Mineral Industries Building, completed in 1929. Home to the Department of Materials Science and Engineering, the new Steidle Building reopened in 2016 with an open concept design featuring shared laboratory space with glass walls. Dramatic displays and murals throughout the building showcase materials discovery and innovations.

CIMP-3D
The Center for Innovative Materials Processing through Direct Digital Deposition (CIMP-3D) is a world-class resource for advancing and deploying additive manufacturing (AM) technology. Located in Innovation Park (230 Building), the 8,000 sq ft facility houses additive manufacturing and hybrid manufacturing systems for polymer, metal, and ceramic materials prototyping, plus characterization instrumentation and a state-of-the-art design studio.

Materials at Penn State Historical Poster Project
The field of materials research is woven from many strands – metallurgy, ceramics, polymer science, physics, chemistry, chemical engineering, electrical engineering, geosciences, the list goes on. The Materials at Penn State Historical Poster Project intends to capture significant people and events related to the illustrious history of materials discovery at this university. The first five metal-print posters in the ongoing series will be on display in the Millennium Science Complex for Materials Day 2017.

About Poster Voting

This year we will be opening a live poll via SMS (text message) on Tuesday, October 17 from 11:00 a.m. – 2:00 p.m. To vote, text your favorite poster number to 850-331-0323. Voting directions are provided in this program and on the poster display. If you want to vote but not via SMS, visit the voting box at the registration desk outside the Nittany Lion Ballroom from 11:00 a.m. – 2:00 p.m.

LIMIT: One vote per attendee.
Poster Listing by Research Category

**Materials Characterization**

1. **Understanding the Native Assembly, Interface Interactions, and Piezoelectric Properties of Cellulose**  
   S. Huang, M. Makarem, I. Chae, S. H. Kim
2. **Electro-Thermal Analysis of β-Ga₂O₃ Based Ultra-Wide Bandgap Schottky Barrier Diodes**  
   B. Chatterjee, A. Jayawardena, S. Dhar, S. Choi
3. **3D Full-Field Mechanical Measurement of Shoulder Bones under Implant Loading**  
   Y. Zhou, G. S. Lewis, A. D. Armstrong, J. Du
4. **Investigation of Surface Conditions on the Cooling of Nuclear Fuel Rods**  
   S. Ebrahim, F. B. Cheung NOTE: THIS POSTER IS DISPLAYED AT #107
5. **Controlling Chemistry and Microstructure for Functional Soft Materials**  
   M. Aplan, J. Litofsky, E. D. Gomez
6. **Resonant Soft X-ray Scattering of Biological Systems**  
   D. Ye, S. Rongpipi, E.D. Gomez, E.W. Gomez
7. **Low-dose Transmission Electron Microscopy of Highly Oriented Polyacetylene**  
   H.-T. Huang, M. D. Ward, S. J. Juhl, A. Biswas, T. A. Strobel, J. V. Badding
   K. L. Knappenberger, Jr., P. J. Herbert, and T. Zhao Second
10. **Defect Phenomena in Nanostructures: An Ultra-high Resolution Electron Microscopy Study**  
    D. Mukherjee, S. Juhl, P. Moradifar, L. Miao, S. Bachu, K. Agueda, N. Alem
11. **In-situ TEM Study on Shape Deformation and Thermal Stability of Silica Opals and Nickel Filled Silica Nano-Opals**  
    P. Moradifar, Y. Liu, J. Russell, T. Mallouk, J. Badding, N. Alem
12. **The High Field MRI Facility at The Pennsylvania State University**  
    T. Neuberger
13. **Research at the Electroactive Materials Characterization Laboratory**  
14. **SNIPe: A Scanning Probe Microscope with In-situ Optical Access for Locating Material and Device Features and Interfaces**  
    L. Pabbi, R. Banerjea, E. Hudson
15. **Using Laser Diagnostics to Understand Changes in Soot Nanostructure**  
    M. Singh, R. Vander Wal
16. **Penn State Underground Pipeline Corrosion “Living” Laboratory**  
    B. Shaw, E. Sikora, C. Van Pelt, K. S. Venkataraman

To vote, text: “#POSTERNo.” to 850-331-0323
### Computer Simulation and Modeling

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<td>Two-Fold Anisotropy in Sodiated Black Phosphorous for Sodium Ion Batteries</td>
<td>T. Chen, P. Zhao, X. Guo, S. Zhang</td>
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<td>Designing and Production of Cork-Based Functionally-Graded Concrete Walls</td>
<td>F. Craveiro, J. Duarte</td>
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<td>Bone Remodeling Under Tooth Loading</td>
<td>K. Su, L. Yuan, J. Du</td>
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126. **National Remotely Accessible Instruments for Nanotechnology (RAIN) Network**

  R. Ehrmann


  S. A. Suliman
Cellulose is one of the most abundant polymers on earth. In plant cell wall, cellulose microfibrils are embedded in other matrix polymers. We focus on understanding the mesoscale organization of cellulose in the cell walls and the interactions between cellulose and other cell wall components by using sum frequency generation/scattering (SFG)/(SFS) vibrational spectroscopy. Also, we investigate the relationship between polar ordering and intrinsic piezoelectricity of cellulose nanocrystals.

SFG is a nonlinear optical process which is sensitive to a media with no inversion symmetry. SFG provides the selective detection of non-centrosymmetric cellulose crystallites without spectral interference from amorphous matrix polymers around them. Using SFG, we are able to investigate the 3D architecture of cellulose organizations including orientation and interfibrillar distances in the intact cell walls without chemical or physical purifications. Our newly developed SFG microscope system with micron-size resolution can also be applied to study cellulose organizations among different plant cell walls. The SFG-microscope helps us to realize the local differences in the packing of cellulose microfibrils. Also, the differences in cellulose deposition in various cell types with distinct roles in plant development can be investigated. Our recent study on plants in different developmental stages has revealed how the packing and orientation of cellulose microfibrils vary in xylem and interfascicular fiber cells as the plant continue its growth.

It has been predicted that cellulose has the piezoelectric properties due to its non-centrosymmetric crystalline structure for several decades. However, the intrinsic piezoelectricity of cellulose has not been measured accurately. It is because no one has provided a solid evidence of polar ordering, which is essential to have the net piezoelectricity. There is no secure method reported to align cellulose crystals in parallel. We are developing SFG vibrational spectroscopy to characterize the polar ordering of cellulose crystals. In addition, we aim to devise effective means to align them in parallel such that the polarity of individual crystals adds up. This will help us elucidating the intrinsic piezoelectric properties of cellulose and contribute to designing cellulose based electro-active devices.
Self-heating is viewed as one major challenge that the Ga$_2$O$_3$ device technology will encounter. The main reason for developing such UWBG power devices is to improve the size, weight, power (i.e., higher power densities), and efficiency over current state-of-the-art GaN and SiC based WBG counterparts. However, the thermal conductivity of β-Ga$_2$O$_3$ is only on the order of 10-20 W/m-K, which is significantly lower as compared to GaN (~150 W/m-K) and SiC (380 W/m-K). Therefore, the self-heating effect in Ga$_2$O$_3$ devices needs to be accurately assessed and managed to accomplish successful transition from the WBG to the UWBG technology in commercial and military power electronics applications and to ensure device reliability.

In this work, for the first time, self-heating in Ga$_2$O$_3$ Schottky barrier diodes (SBD) has been investigated using non-invasive, in-situ optical techniques and multi-physics simulation. Thermoreflectance thermal imaging and infrared thermography were used to probe the device surface temperature. The device peak temperature that occurs in the vicinity of the resistive Schottky contact was measured via cross-sectional Raman thermography. Experimental results were validated through comparison with 3-D coupled electro-thermal simulation. The collected data and simulation results indicate that without optimized thermal design, the temperature rise of a Ga$_2$O$_3$ SBD can be an order of magnitude higher than that for GaN and SiC based vertical diodes under forward biased operation with identical areal power dissipation. Simulation shows that the Ga$_2$O$_3$ technology allows significant reduction of the device volume to achieve a rated blocking voltage for commercial SiC power diodes. However, the thermal concern still remains that needs to be overcome through employing proper thermal management schemes.

### 3D Full-Field Mechanical Measurement of Shoulder Bones under Implant Loading

Y. Zhou, G. S. Lewis, A. D. Armstrong, J. Du

The mechanics of shoulder bone under implant loading is important to the success of shoulder bone implant treatment. This work presents the results of a noninvasive three-dimensional (3D) full-field mechanical measurement of shoulder bones under implant loading conditions. Glenoid implants are placed in human cadaver specimens and loaded. Micro X-ray Computed Tomography (µ-XCT) of the specimens are taken under no-load and loaded conditions. Using image processing technique and digital image correlation in 3D, the 3D displacement and strain field inside the shoulder bone are calculated. The results are displayed using 3D visualization tools. The clinical implications of the results are discussed for the improvement of glenoid implant treatment.

### Investigation of Surface Conditions on the Cooling of Nuclear Fuel Rods

S. Ebrahim, F. B. Cheung

NOTE: THIS POSTER IS DISPLAYED AT #107

This research investigates the influence of surface conditions on the cooling process of nuclear fuel rods. Specifically, material characterization of CRUD formed on the fuel rod surfaces is performed and its effects on the cooling of fuel rods are studied. The term CRUD (Chalk River Unidentified Deposits) is used to describe the deposited corrosion products on the surface of the fuel cladding rods during the operation of Pressurized Water Reactor (PWR). The Pennsylvania State University has constructed and operated a 7 x 7 rod bundle test facility under the Rod Bundle Heat Transfer (RBHT) Program sponsored by United States Nuclear Regulatory Commission (NRC). Inconel type 600 rods with the dimensions of 9.5 mm diameter and 3.657 m heated length are used in the test facility. They have experienced an approximate of 200 total heating and cooling cycles under system...
pressure and cladding temperature ranges between 0.138 – 0.414 MPa and 315 – 1093 °C, respectively.

Material characterization has been performed on test samples collected at different elevations of the heated rods to identify the microstructures of the CRUD layers by using field emission scanning electron microscopy (FE-SEM), scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDS), and x-ray diffraction (XRD). Additionally, an automated goniometer and optical profilometry are used to measure, respectively, the surface roughness and the water contact angle of selected rod surfaces with and without CRUD formation. The goal is to correlate the surface conditions of the rods such as the surface roughness, the water contact angle, and the thickness, porosity and chemical composition of the CRUD layer on the cooling behavior of the rods under PWR accident conditions. A heat transfer correlation has been developed from the data which predicts the enhancement of the cooling process of the fuel rods following a severe accident such as loss-of-coolant-accident (LOCA) resulted in improving the safety of the PWR.

5
Controlling Chemistry and Microstructure for Functional Soft Materials

M. Aplan, J. Litofsky, E. D. Gomez

The research focus of the Gomez group is on understanding how structure at various length scales affects macroscopic properties of soft condensed matter. Though diverse, complex organic molecules share free energy landscapes dominated by non-equilibrium states and a theme of disorder. Understanding the fundamental processes that lead to, for example, charge transport and separation, requires characterization of equilibrium, near equilibrium, and far from equilibrium structures.

Current efforts are directed at understanding the structural parameters that affect the performance of organic electronics, including solar cells and transistors, through a combination of electron and light microscopy, X-ray and light scattering, electron diffraction, and device testing. Through model systems, we study the physics of charge injection and charge transfer at semiconductor-metal interfaces as well as organic heterojunctions. Furthermore, we examine the microstructure of polymeric membranes used in water filtration to uncover how membrane performance depends on structural properties. We are also extending our structural characterization tools for the study of biological systems, including proteins, viruses, and plant cell walls.

6
Resonant Soft X-ray Scattering of Biological Systems

D. Ye, S. Rongpipi, E.D. Gomez, E.W. Gomez

The structure at one to a few hundred nanometers is critical to the properties and functionality of proteins, lipid membranes, hydrogels, and a variety of complex biological assemblies. Small angle X-ray scattering is a powerful tool capable of probing the aforementioned length scales, but is often limited by the relatively small differences in electron density between phases or domains of soft materials. Resonant soft X-ray scattering (RSOXS), a technique developed within the last decade for the study of polymeric thin films, couples spectroscopy and scattering to overcome some of the critical limitations of hard X-ray scattering. Conventional X-ray scattering relies on circa 8 keV X-rays as the incident radiation; in contrast, RSOXS employs X-ray energies between 0.2 and 1.5 keV to access various absorption edges (e.g., C, N, O, F, Ca) and enhance scattering contrast. Working at these lower energies, however, requires a high-vacuum sample chamber. We have been taking advantage of recent advances in wet-cell
technology for transmission electron microscopy experiments to enable RSOXS of biological materials in solution, thereby opening the door for extracting chemical contrast from multicomponent biological assemblies. We have demonstrated proof-of-concept experiments using wet-cell RSOXS to extract the envelope function of proteins. Furthermore, we have used RSOXS to examine the structure of plant cell walls, where we extract the average spacing between cellulose nanofibrils.

### 7

**Low-dose Transmission Electron Microscopy of Highly Oriented Polyacetylene**

H.-T. Huang, M. D. Ward, S. J. Juhl, A. Biswas, T. A. Strobel, J. V. Badding

Recent advances in the synthesis of polymeric fibers and textiles have demonstrated that well-defined supramolecular architectures with desired mechanical and electronic properties can be designed and produced at a massive scale. In order to understand the structure-property relationship of these polymeric fibers, characterization techniques in the subnanometre scale is critical because the macroscopic properties of these fibers are usually closely related to the local atomic structures and chemical functionality. However, direct observation of the atomic structures of polymeric fibers through electron microscopy remains a challenge as these soft materials are usually very sensitive to electron beam damage.

Polyacetylene is a well-known electrically conducting linear organic polymer with *cis-trans*-isomerism. The ratio of *cis*- and *trans*-isomers in the material has a critical impact on the properties. Using low-dose transmission electron microscopy and microanalysis technique, we identified highly oriented polyacetylene (HOPA) synthesized via high-pressure induced solid-state polymerization is primarily composed of *trans*-isomers. Furthermore, the structural transformation of HOPA film into nanocrystalline buckydiamonds (onion-like graphitic shells with diamond cores) under electron beam radiation was examined through high-resolution transmission electron microscopy (HRTEM) and Electron Energy Loss Spectroscopy (EELS). Such low-dose microscopy and microanalysis techniques open up a wide variety of opportunities in characterizing beam sensitive materials such as carbon nanomaterials, synthetic polymers, and biological fibers, which can potentially offer insights that cannot be provided by conventional analytical chemical methods.

### 8

**Photonic Nanomaterials Examined Using Magneto-Optical Correlative Light and Electron Microscopy (MO-CLEM)**

K. L. Knappenberger, Jr., P. J. Herbert, T. Zhao Second

Correlative light and electron microscopy (CLEM) is a powerful approach to developing structure-function relationships for nanoscale materials. Our group has developed nonlinear optical (NLO) imaging methods that can be used to pinpoint the location of an optical point source with one-nanometer transverse and ten-nanometer axial localization accuracies. Among the suite of NLO processes, magneto-optical (MO) methods enable simultaneous spatially resolved characterization of the electronic and optical properties of these material domains. We will provide examples using variable-temperature, variable-magnetic-field optical methods to determine electronic *g* factors, term symbols, and zero-field energy gaps for excitonic transitions in nanoscale materials.
As an alternative clean energy source, proton exchange membrane (PEM) fuel cells are a promising technology; however, the high cost of noble-metal catalysts (platinum) hinders its widespread commercialization. Contrarily, anion exchange membrane (AEM) fuel cells employ cationic moieties fixed to polymer chains and do not require noble-metal catalysts. However, AEMs have their own set of challenges, such as substandard stability and conductivity. Work in the Hickner group has focused on synthesis/characterization of a more stable AEM, and evaluation of water/polymer interactions in AEMs to better understand ways of improving AEM conductivity.

A series of comb-shaped quaternary ammonium-containing poly(2,6-dimethyl-1,4-phenylene oxide) (QA-PPO) were synthesized with different lengths of alkyl side chains, where Cy refers to length \( y = 6, 10, 16 \) and D40 to degree of bromination (0.4 bromomethyl groups per PPO unit). Specifically, benzylidimethylhexyl ammonium (C6D40), benzylidimethyldecyl ammonium (C10D40), and benzylidimethylcetyl ammonium (C16D40). Also synthesized was benzyltrimethyl ammonium (BTMA) to serve as a QA-PPO control without side chains.

Solubility studies of the QA-PPOs exhibited excellent solubility in pure methanol, ethanol and \( n \)-propanol, and insolubility in pure water (even at 80°C), demonstrating their usefulness as catalyst layers. Small-angle X-ray scattering analysis revealed ionic peaks (indicating ionic clusters due to nanophase separation) of a moderate size for BTMA40, C6D40 and C10D40, but a distinguishable peak for C16D40. Water uptake studies displayed a lower water uptake relative to the longer alkyl chain length of the comb-shaped polymers; C16D40 was the most hydrophobic with restricted water absorption. Hydroxide conductivity measurements showed higher conductivity relative to the longer alkyl chain length of the comb-shaped polymers compared to BTMA40. Alkaline stability studies of the comb-shaped QA-PPOs demonstrated a slow decline in conductivity during the initial 200 h of fast degradation. After 2000 h of immersion in 1 M NaOH at 80°C, they retained ~80% of their conductivity, while the BTMA40 decreased to 40%. Overall findings suggest that their comb-shaped architecture is a promising approach for AEM design.

QA-PPO membranes were saturated with sodium azide and resulting spectra were measured in attenuated total reflectance (ATR) Fourier transform infrared (FTIR) configuration from 0 to 90% relative humidity. The hydration-sensitive azide (\( N_3^- \)) asymmetric stretch peak was monitored in-situ during hydration experiments. QA-PPO samples had different interactions with azide species as evidenced by the position and intensity of their characteristic FTIR bands. In BTMA40, the wavenumber of the \( N_3^- \) group was located at 2002 cm\(^{-1}\) and 2022 cm\(^{-1}\) at 0% RH and 90% RH, respectively. For the comb-shaped samples, the \( N_3^- \) absorbance was observed at approximately 2000 cm\(^{-1}\) and 2017 cm\(^{-1}\) at 0% RH and 90% RH, respectively. Results indicated that polymer interactions with water became
weaker as the alkyl pendant was longer. The resulting shift was associated with the dynamic hydrogen-bonding environment inside the polymer membrane, and to cationic interactions with the azide ion. The azide probe was successful in evaluating water/polymer interactions and effectively measured by ATR-FTIR.

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Defect Phenomena in Nanostructures: An Ultra-high Resolution Electron Microscopy Study
D. Mukherjee, S. Juhl, P. Moradifar, L. Miao, S. Bachu, K. Agueda, N. Alem

The atomic and chemical structure of materials can have a profound effect on the resulting physical, chemical, and mechanical properties and lead to applications in electronics and optoelectronics, energy, and catalysis. Probing and understanding the effect of defects, vacancies, interfaces, grain boundaries, and domain walls on the chemical, physical, and electronic properties of materials is a crucial step in material nano-engineering. We use ultra-high resolution aberration-corrected transmission electron microscopy to visualize the atomic structure, electronic structure, bonding, and chemistry in a wide variety of nanocrystals atom-by-atom in both static and dynamic mode. This presentation will show the structurally-driven chemical, physical, and electronic properties by probing the atomic bonding, registry, and chemistry using a variety of electron microscopy imaging and spectroscopy techniques. The focus of our current research is mainly on complex oxides, van der Waals heterostructures, heterojunctions, metalattices, and other novel nanostructures synthesized under extreme conditions.

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In-situ TEM Study on Shape Deformation and Thermal Stability of Silica Opals and Nickel Filled Silica Nano-Opals
P. Moradifar, Y. Liu, J. Russell, T. Mallouk, J. Badding, N. Alem

Metalattices are three-dimensional interconnected ordered arrays of nanostructured solids with periodicity size range between 1 nm – 100 nm. Functional properties of 3D ordered frameworks such as nano-opals and zeolites can be tuned by infiltrating them with semiconductor materials (like Si, Ge etc) and/or metals (Pt, Ni, Ag etc). The quantum confinement in these metallic nanostructures, such as Ni infiltrated nano-opals, results in an equal length scale of the intrinsic electron mean free path and magnetic characteristic length which can lead to a strong interaction between the intrinsic physical and structural parameters resulting in novel magnetic, electric and thermal behavior. Using in-situ heating high-resolution scanning/transmission electron microscopy (HR-S/TEM) techniques, we aim to understand structural changes, thermal stability, and thermophysical behavior of silica nano-opals and Ni filled silica nano-opals before and after infiltration as a function of the size of the silica nano-opals and temperature. This study will present the structural and chemical changes that occurs in Ni infiltrated silica opals under heating conditions. Morphology changes occurring at different temperatures are visualized by TEM. Imaging the structural and chemical changes of silica nano-opals and Ni filled nano-opals and understanding the thermal stability and thermophysical behavior under heating conditions can provide information on high temperature magnetic behavior of this material as a function of both temperature and size of the silica nano-opal templates as a 3D ordered template. This understanding is the key to develop novel metalattice materials for future high temperature magnetic and electronic applications.
Magnetic Resonance Imaging (MRI) is a versatile tool to image noninvasively. Its excellent soft tissue contrast in in vivo imaging makes it an indispensable tool in diagnostics in the daily clinical routine. Nevertheless, MRI can do so much more. Besides the in vivo imaging MRI can be used e.g. to monitor moisture distribution in drying concrete, dried organic materials like coffee beans, or wood. It can also be used to quantify the lipid distribution in objects like seeds which is an essential component to the biofuel and the crop research community. Furthermore, the development of new multimodal ‘theranostic’ nanoparticles in cancer research is one of our research projects as well as the design and the construction and testing of new magnetic resonance radio frequency detectors. Many of these projects are developed in cooperation with faculty from several departments, especially with the faculty from the Materials Research Institute.

The High Field Magnetic Resonance Imaging (MRI) Facility at the Pennsylvania State University comprises two high field preclinical imaging systems. The 7 tesla system is a recently upgraded Bruker Biospec with the newest technology for preclinical imaging and spectroscopy. It has 4 receiver channels, x-nuclei capabilities and the latest available software. The second system is a 14 tesla microimaging system from Agilent. With its four receiver channels and the x-nuclei capabilities, it is a versatile instrument to acquire high resolution data.

Research at the Electroactive Materials Characterization Laboratory (EMCLab) focuses on processing-microstructure-property relationships in polymer-based smart materials. Our goal is to develop materials exhibiting unique combinations of mechanical, electrical and coupled properties for sensing, actuation, and energy storage. Our current projects cover the range below:

- Polymer nanocomposites: polymer nanocomposites are promising candidates to overcome the limitations of monolithic materials; significant improvement levels can be achieved by incorporating high surface area particles in polymer matrices. Chemically modifying the nanoparticles leads to the ability to tune the expansive surface area and therefore dramatically enhance the effective properties using very low particle contents. Additionally, we demonstrate that manipulation of the particles using mechanical and electric fields is a big step towards spatially engineering and designing material systems for prescribed performance.
- Active fiber composites (AFCs) for sensing and actuation: AFCs are long circular piezoelectric ceramic fibers embedded in an epoxy polymer, where the electric field lines are parallel to the fiber direction instead of through-the-thickness. AFCs can be used in several applications for self-health monitoring, vibration control and energy harvesting. Full experimental characterization of the commercial composites and finite element modeling with parametric study on the design parameters are conducted in order to maximize the performance of new flexible electro-active composites.
- Multi-field responsive origami-inspired structures: The objective is to develop multi-field active materials yielding on-demand large bending and folding. A variety of electroactive polymers and polymer nanocomposites are being developed and investigated to realize active origami-inspired
structures using a combination of experimental materials development, analytical and FEA modeling and multiscale characterization.

- Polymer composite for low dose nuclear threat detection: A novel approach is being developed to actively detect shielded special nuclear materials (SSNM) while in transit with a relocatable low dose system. Several composite detectors composed of a poly(vinyl) toluene as the scintillating matrix and GS20 lithium glass in different geometries are being manufactured and characterized.

- Multilayer polymer laminates for high energy density and low loss dielectrics: The objective of this project is to study the breakdown behavior of multilayered polymer laminates under pulsed conditions and at low and high temperatures. Findings will inform the development of novel polymer-based capacitors with high dielectric permittivity, low dielectric loss and high energy density. An important expected outcome is that the multilayered laminates will enhance capacitor and cable reliability at high temperature because dielectric failure paths are deflected at the many interfaces due to barrier effects.

- Polymer surface modification: Two ways to modify the chemically inert polymer surface are studied in our group: plasma treatment and molecular layer deposition (MLD). Plasma treatment offers tailorable modification of the polymer surface by modifying the surface chemical bonds, adding species such as polar and/or functional groups, and forming radicals. Molecular layer deposition enables creating organic coatings on polymer substrates. The main objective of these projects is to develop a comprehensive understanding of the electronic transport and polarization phenomena at resulting dielectric interfaces created by etching the surface by plasma or depositing an organic layer by MLD.

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SNIP: A Scanning Probe Microscope with In-situ Optical Access for Locating Material and Device Features and Interfaces

L. Pabbi, R. Banerjea, E. Hudson

Scanning Probe Microscopy (SPM) has proven to be a powerful tool in studying exotic materials by measuring, with atomic resolution, topographic and electronic properties. We present here a new variable temperature (4K–RT), low noise SPM that combines atomic force (AFM) and scanning tunneling (STM) capabilities. In addition, our novel optically-guided tip positioning system allows us to initially position the tip over specific features in large (5 mm) samples with high precision (10 µm) before resorting to “step-and-scan” techniques. This ability makes our system especially attractive for studies of small or rough crystalline samples, dispersed two-dimensional flakes, and interfaces. Coupled with a suite of sample preparation techniques such as Ar-ion sputtering, annealing and variable temperature sample cleavage, we can accommodate a wide range of crystalline and non-crystalline samples and devices for atomic resolution studies.
Particulate matter such as soot derived from vehicle emissions or other combustion processes is detrimental to human health. Deteriorating air quality due to particulate emissions has been linked to high risk of heart and lung diseases and also contributes to climate change. Thus, to establish global air quality guidelines, it is important to measure the concentration of soot in the atmosphere. Laser induced incandescence (LII) is one such diagnostic that measures soot concentration and primary particle size. This technique can be used in-situ and has high sensitivity, providing accurate measurements even with low concentrations of soot. In order to interpret the LII signal for these measures requires reference to models for LII based on an energy balance. These models predict soot primary particle size and concentration, each with a set of assumptions about soot physical parameters – often leading to discrepancies between simulated and experimental results. This work uses carbon black as soot surrogate and highlights some such differences by comparing experiments with model predictions. For instance, transmission electron microscopy (TEM) from this work shows significant changes in carbon black nanostructure upon laser heating, analogous to annealing, an aspect overlooked by LII models. UV-Vis spectroscopy of laser annealed carbon black shows that its emissivity can be approximated by that of a black-body with unit emissivity. This makes the analysis of the LII signal more straightforward than with presumed initial properties. By not accounting for such changes, models often over- or under-predict soot primary particle size when compared to particle sizes directly measured by TEM imaging. Concentration determination is similarly skewed. Thus, refinement of model parameters by comparison to experimental results is required to better predict these quantities – as shown by the presented results.

The concept is a living laboratory for studying underground corrosion and pipeline corrosion control. This facility would realistically approach the unique challenges present in assessing pipeline corrosion and coatings damage and implementing and designing better and more cost-effective cathodic protection systems for the control of underground corrosion. To date, the living laboratory has been using existing Penn State underground infrastructure that is cathodically protected (buried tanks/ gas pipelines and above ground storage tanks) for teaching concepts of underground corrosion control. We would like to expand our capabilities by building a small, low-cost underground test field of buried empty, capped pipe segments with “seeded” defects and other pipeline corrosion control challenges to aid in the research and development of new inspection techniques, new corrosion protection products, and provide a platform for a broad range of training opportunities. This facility would offer hands-on learning experiences for students, a new research avenue to solve problems that are currently relevant to the pipeline industry, a facility for pipeline professionals to practice their current skills while interacting with PSU students and faculty, a platform to discuss current and future pipeline industry needs and research, training of industry-ready professionals, and the chance for community outreach and education. This facility will take advantage of PSU’s broad expertise in the science and engineering needed for development of new inspection techniques and tools and data analysis (corrosion data informatics).
A to-be-released commercialized phase-field package μ-pro (microstructure-property modeling package) and its academic counterpart MesoExplorer are presented for modeling microstructure evolution and predicting material properties in a variety of material systems and devices. Both packages, at heart, are a series of phase-field models implemented with modern Fortran and MPI, thus gaining native numerical and performance advantages. The packages excel in dealing with numerous types of problems, e.g., material response to an external field and effective material properties (mechanical, thermal, transport, piezoelectric, dielectric, etc.) of an arbitrary single-phase or multi-phase microstructure; domain structure and domain switching in ferroelectric, magnetic, ferroelastic and multiferroic systems and devices; dielectric degradation and breakdown in capacitors; microstructure evolution during structural and diffusional phase transformations, Ostwald ripening and grain growth in alloys; ion transport and microstructure evolution in lithium ion batteries and solid oxide fuel cells. Users can easily finish the whole modeling procedure, from parameter input to program execution and output visualization, with a combination of command line interface and graphical user interface. Such versatile phase-field-based packages would be helpful for studying and designing materials and devices for desired properties.

Dr. Long-Qing Chen’s group focuses on modeling the thermodynamics and kinetics of phase transformations and multi-scale microstructure evolution. We study bulk and thin film materials using multi-scale computer simulations combining the first-principles calculations and phase-field method. One can use the phase-field method to help interpret as well as provide guidance to experiments. Our group collaborates extensively with experimentalists around the world, industry, and national labs.

Phosphorous represents a promising anode material for sodium ion batteries and is regarded as the counterpart of Si for lithium ion batteries. Recent in-situ transmission electron microscopy studies evidenced anisotropic swelling in sodiated black phosphorous. We rationalize that the apparent anisotropic swelling may be originated from two intrinsic anisotropic properties inherent to the layered structure of black phosphorous: sodium diffusional directionality and insertion strain anisotropy. To assess the role of the two-fold anisotropy in morphological evolution and stress generation upon sodiation, we develop a chemo-mechanical model by incorporating the intrinsic anisotropic properties with large elasto-plastic flow in sodiated black phosphorous. Our modeling results reveal that the apparent morphological evolution is critically controlled by the coupled effect of the two intrinsic anisotropic properties. In particular, sodium diffusional directionality generates along the [010] and [001] directions sharp interphases, which constrains anisotropic development of the insertion strain. The coupled effect renders substantial difference in sodiation induced stress generation when sodiation starts from different crystal facets. In addition to providing a powerful modeling framework for sodiation or lithiation of layered structures, our findings shed significant light on the sodiation-induced chemo-mechanical degradation of black phosphorous as a promising anode for the next-generation sodium ion batteries.
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<td>20</td>
<td>Designing and Production of Cork-Based Functionally-graded Concrete Walls</td>
<td>F. Craveiro, J. Duarte</td>
<td>Natural systems are optimized for the loading conditions they are subjected to, and their geometry and material properties change according to stress or strain requirements. Current Additive Manufacturing technologies consider the design and fabrication of physical elements with homogeneous material properties, not heterogeneous composite materials with varying material distribution, called functionally-graded materials (FGM). With FGMs it is possible to take into account different functional requirements in the design, simulation, and fabrication of construction elements, optimized for specific thermo-mechanical conditions. In this work, we present a new strategy developed to optimize material composition, using a graphical algorithm editor together with FEM software. The proposed algorithm adjusts the multi-material ratio locally, according to the stress map, simulating nature’s structural behavior. The material is then produced using an additive manufacturing process developed for this purpose, which combines a robotic arm and concrete mixers and pumps.</td>
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<td>21</td>
<td>Bone Remodeling under Tooth Loading</td>
<td>K. Su, L. Yuan, J. Du</td>
<td>The stability and success rate of orthopedic and dental implants are affected by their surrounding bone quality. Bone adapts to mechanical loads through remodeling activities to achieve new equilibrium in strain/stress state. The object of this study is to develop a numerical algorithm to simulate bone remodeling activities under mechanical loading. Finite element method is used to calculate the strain/stress distribution in the alveolar bone under tooth/implant loading. The bone density remains unchanged near the equilibrium point of the mechanical stimulus; under greater or smaller mechanical stimulus, it increases or decreases. Iterations are performed to simulate the evolution of bone density due to mechanical stimulus. The effects of model geometry and the adjacent teeth are studied. The effects of various applied loads and different boundary conditions are also compared. The calculated results are validated using computed tomography (CT) data of human mandibles. The implications of the results on patient-specific treatment and the insights for clinical techniques are also discussed.</td>
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<td>22</td>
<td>DFT Studies of Intermetallic Gamma-Brass Crystal Structures for Selective Hydrogenation</td>
<td>H. He, A. Dasgupta, G. Kumar, R. M. Rioux, M. J. Janik</td>
<td>Bimetallic compounds can offer tunable site electronics and ensemble structure for selective hydrogenation catalysis. In this study, we consider the γ-brass phase (Cu$_2$Zn$_8$ prototype) in order to expose surfaces with controlled M$_x$ nuclearity to control the selectivity for hydrogenation. The γ-brass structure has a 52 atoms unit cell with 4 distinct symmetry sites — outer tetrahedral (OT), inner tetrahedral (IT) octahedral (OH) cuboctahedral (CO). In particular, the Pd-Zn γ-brass atomic arrangement as well as the substitution pattern of Zn by Pd in the Pd-Zn γ-brass phase (15.4-24%) has been extensively studied by Edstrom and Westman through x-ray diffraction analysis. Surface energy calculations indicated that the most stable Pd$<em>9$Zn$</em>{44}$ facet is (1-1 0), which exposes only monomers for Pd$<em>6$, but includes Pd trimers for Pd$</em>{9,11}$. We vary the number of Pd atoms per isolated active site and investigate its effect on H$_2$ dissociation and acetylene hydrogenation mechanisms. DFT calculations agreed with experimental results that H$_2$ activation is faster on trimer sites, substantiating the formation of Pd$_3$ trimer sites on Pd$<em>3$Zn$</em>{44}$ catalyst surfaces. The activation barrier for H$_2$ dissociation is nearly identical experimentally on Pd9, Pd10 and Pd11, further substantiating the isolation of the Pd trimer sites. DFT calculations indicate that acetylene binds strongly on both monomer bridge and trimer sites, whereas ethylene binds strongly on monomer</td>
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atop and trimer side atop sites. At the same time, H₂ dissociation and binding adjacent to ethylene is only possible on the trimer sites. DFT calculations showed the apparent barrier of ethylene hydrogenation is higher than the ethylene desorption barrier, which indicates Pd₈Zn₄₄ is superior catalyst in selectively hydrogenating acetylene to ethylene. Pd₉ on the other hand, contains trimers on the surface, which can lower the ethylene hydrogenation barrier, compared with Pd₈Zn₄₄. The full path of acetylene hydrogenation on these isolated sites, as well as a microkinetic model for acetylene hydrogenation on these intermetallics, will be presented. The gamma-brass intermetallic structures offer isolated active sites with controlled nuclearity, allowing both the design of active and selective catalysts as well as the elucidation of site requirements.

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Predicting Stability of Modified Metal Oxide Surfaces with Functional Atomic-Layers for Nano-engineered Catalysts

A. S. M. Jonayat, A. van Duin, M. Janik

Multicomponent metal oxide systems can offer tunable redox properties and chemical reactivity. These materials are used in fuel cells, gas sensors, and as heterogeneous catalysts. The large number of possible combinations of different mixed-metal oxides and their metastability make the experimental discovery of such systems very inefficient. We focus on predicting the (meta)stability of two classes of these materials with potential for unique chemical properties - (1) Monolayers of oxidized transition metals over another metal oxide support (2) Surface-confined mixed oxides. For monolayer metal oxides, we present an ab initio thermodynamic framework using density functional theory to accelerate this discovery process by predicting stable monolayer metal oxides that can be subjected to further computational study or experimental investigation. As an example of the application of this framework, we present our stability analysis of ZnO (0001)-Zn terminated and rutile TiO₂ (110) surfaces with epitaxial M₂O₇ (M=Pd, Ru, Ni, Pt, Au, Zn) monolayers. Metastability is predicted relative to segregated particle structures of varying radii. We predict that NiO can form a metastable monolayer with the same stoichiometry as the support, ZnO (0001)-Zn. A PdO and RuO₂ monolayer on ZnO (0001)-Zn are potentially stable. A monolayer of RuO₂ on TiO₂ (110) is stable relative to segregated RuO₂ particles of 2 nm radius or less. However, RuO₂ shows a high preference for growing as 2D multilayer islands. Predicted stable monolayers are also found stable against subsurface segregation in the host oxide. For surface-confined mixed metal oxides, as a model system, we examined stability of mixed metal oxides of Fe₂O₃, Cr₂O₃, V₂O₃ on their (0001) surface termination. We show that pure oxide surface stability is a descriptor of the surface segregation preferences for these systems. Using thermodynamic relationships, we predict transition points for these surface-confined mixed metal oxides at which exchange between surface/subsurface and subsurface/surface metal atoms occur due to varying oxygen chemical potential.
Electrochemical energy storage is dominated by batteries and supercapacitors; batteries exhibit high energy capacities but low charging rates, whereas supercapacitors are characterized by fast charging times but low energy densities. The development of advanced technologies combining the energy density of batteries with the power density of supercapacitors is critical to overcome the frontier separating the performance of electrochemical systems from that of internal combustion engines and meet the technical requirements for electric transportation and grid energy storage. A subset of supercapacitors, known as pseudocapacitors, are energy devices characterized by fast and reversible redox reactions near the surface of the electrode. Studying pseudocapacitive processes requires one to consider the time-dependent evolution of the electrolyte at the electrified interface. Although this problem can be tackled by leveraging the accuracy of first-principles molecular dynamics, these simulations are computationally demanding, making it challenging to apply them to the combinatorial discovery for pseudocapacitive oxides. We simulate the response of pseudocapacitive electrodes under electrochemical conditions through the use of electronic-structure methods used together with a self-consistent continuum solvation method to build an extensive dataset of free energies as the surface of the material is gradually covered with ions under applied voltage. This dataset is then combined with grand-canonical Monte Carlo sampling to compute adsorption isotherms and charge–voltage responses. The combination of these two methods allows them to identify the factors that endow them with their exceptionally high charge capacity with an initial focus on ruthenium dioxide as a prototypical material. Our approach provides a widely applicable quantum–continuum framework to predict the intrinsic properties of pseudocapacitive oxides and ultimately optimize their charge storage performance.

This poster presents a brief introduction of Phases Research Laboratory advised by Prof. Zi-Kui Liu at the Department of Materials Science and Engineering. Our research activities in computational materials system design are financially supported by different organizations, i.e., National Science Foundation (NSF), industries, DARPA, U.S. Army Research Laboratory (ARL), U.S. Air Force, and other National Laboratories (i.e., NETL), NASA Jet Propulsion Laboratory (JPL). We briefly describe and greatly appreciate the support, which also shows the various opportunities/collaborations for our current and potential group members. The main methodologies applied in our multi-scale modeling works are graphically described. Under the support of CALPHAD committee and Bayer Travel Fund (International Travel Grants for iMATSE Graduate Students at PSU), we show a great amount of international travel chances for our group members to attend international workshops, conferences, and exchange opportunities studying abroad.
We present four research lines in our group. They all have in common the use of Quantum Mechanics to model the properties of materials: 1) The control of ground state symmetries using electric fields in the Landau levels of bilayer graphene. 2) The energetics of the formation of inversion domains in polar GaN. 3) The dynamics of protons adsorbed on alumina surfaces. 4) The evaluation of the conductivity of graphene with static impurities.

G. DuCharme, B. Green, J. Robins, M. Umar, J. Sofo

Our group develops and applies novel computational tools to predict and improve the properties of next generation energy conversion and storage materials. Our research team operates at the frontiers of materials science, physical chemistry, applied mathematics, and computer science. We aim to break down the complexity of material problems in order to guide the development of future energy materials. Central to this work is the development of quantum-continuum methods that provide an accurate and computationally efficient description of the electrode-solution interface. The quantum-continuum approach permits the systematic study of interfacial phenomena for electrodes in contact with electrolytic environments under an applied bias. Coupling this method with advanced statistical mechanical tools and Monte Carlo sampling techniques facilitates the finite temperature description of a broad class of electrode-solution interfaces. Our group applies these methods to study electrodeposition phenomena on transition metal surfaces, energy storage mechanisms at pseudocapacitive interfaces, as well as photocatalytic water splitting for hydrogen production at semiconductor-solution interfaces.

The first isolation of graphene in 2004 has led researches on two-dimensional (2D) atomic crystals into a vast field over the last decade. In parallel with the greatly expanding 2D library ever since, tremendous developments in the synthesis and understanding of two-dimensional materials such as graphene, phosphorene, BN and MoS2 have spurred great interest in exploiting their three-dimensional (3D) heterostructures through layer-by-layer stacking, where van der Waals (vdW) interactions emerge as a versatile ‘weak glue’ keeping the stack together. With rationally chosen building blocks (2D crystals) and stacking sequence, these 3D heterostructures may compensate for the weakness of its constituent 2D crystals and possess exceptional multifunctionalities that enable multi-tasking (mechanical, optical and electronic) applications. Despite such inspiring progress and promising designing, defects have been seen as imperfections that degrade device performance and layered systems are particularly rich in this regard. For one thing, because of the relatively low out-of-plane rigidity of such 2D crystals, ripples can be easily formed during stacking. Our recent research has shown such line defects, termed as riplocations, are very straight, narrow, and crystallographically oriented. For another, due to the lattice mismatch among neighboring layers of different crystals species or/and orientations, the
coincidence Moire superstructures would thus originate, in parallel with strong, localized interactions.

On one hand, to further investigate such fundamental stacking mechanism and its effect in an extending length scale, we present a simple and effective quasi-continuum model using finite crystal method based on the exponential Cauchy-Born rule. For each graphene-like crystal specie, a homogenized finite crystal model is developed exclusively, by fitting its unique lattice parameters and moduli. In addition, to catch the effect of both registry and lattice mismatch, a modified van de Waals interaction model is implemented accordingly. Our study has shown that the model is effective in not only charactering the morphology, stability, motion, and interaction of rippllocations but also uncovering the highly localized stress due to registry and lattice mismatch. On the other hand, we present here an approach called diffusive molecular dynamics (DMD), which can capture the diffusional time scale while maintaining atomic resolution by coarse-graining over atomic vibrations and evolving a smooth site-probability representation.

Spatial and temporal control for deep tissue regeneration is largely dependent on the precise targeting of therapeutics to progenitor cells at the site of the defect, as well as properties of drug delivery vehicles used to affect the intended area. Here we present our efforts to develop a targeted RF stimulated siRNA delivery tool to modulate tissue regeneration via spatiotemporal control of post-transcriptional gene regulation. To this end, we have developed a heterodimeric Au-Fe₃O₄ nanoparticle composed of gold and iron oxide subunits that allow for discrete chemical attachment sites and chemistry for dual functionalization with targeting molecules and miRNA mimics, in this case Anti-CXCR4 antibody and miR-148b mimic respectively. To control activation (uncaging) of the miRNA mimic, we have developed a stimulus responsive Diels-Alder linker which tethers the oligo to the surface in an inactive state. The Diels Alder linkage provided an effective spatial and temporal control switch to modulate gene expression via radio frequency (RF) activation, while Anti-CXCR4 antibody provides specific targeting of heterodimer NPs to hBMSCs. Regarding targeting of therapeutics to progenitor cells, MALDI demonstrated effective conjugation of the Anti-CXCR4 antibody to the iron oxide portion of the AuFe₃O₄. Flow cytometry confirmed attachment of the Anti-CXCR4 antibody to the hBMSCs. Osteogenic hBMSCs exhibited upregulation of alkaline phosphatase (ALP) at day 7, as well as calcium deposition at 14 and 21 days when stained with Alizarin Red and further supported by ICP-AES analysis for the gold, iron, magnesium, phosphorous, and calcium. With demonstrated upregulation of hBMSCs osteogenesis and preferred targeting of NP to hBMSCs in vitro, using this approach opens the possibility for deep tissue regeneration and repair for future studies.

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Specific Targeting of hBMSCs and RF Mediated Osteogenesis Using Dumbbell Shaped AuFe₃O₄ Nanoparticles Conjugated with Anti-CXCR4 Antibody and miR148b Mimic

Self-assembly of Smart Multifunctional Hybrid Compartments with Programmable Bioactivity

G. Cheng, S. Hao, Y. Wan, S.Y. Zheng

As one of the basic building units of life, the cell is a compartmentalized space with an outer membrane and multiple internal organelles, which can mediate many complex biochemical reactions in concert and provide specialized cellular functions. By mimicking biological compartmentalization, the design and construction of the smart artificial microcompartments are highly desirable for understanding the mechanism of formation of primitive cells for the origin of life and have technological effects in broad fields such as materials science, catalysis, environmental remediation, biomedicine, and biotechnology. However, it remains a critical challenge for the construction of a structurally stable, semipermeable, and a multifunctional compartment that can maintain a protective and confined internal space while allowing internalization of ingredients. Here, we present a strategy for construction of novel smart multifunctional hybrid compartments (SMHCs) with semi-permeability, stimulus-response, and enzymatic bioactivity.

Portable Sample-to-Answer Multiplexed Molecular Diagnosis for Malaria in Remote Areas

G. Choi, T. Prince, J. Miao, L. Cui, and W. Guan

This paper reports a multiplexed “sample-in-answer-out” diagnostic system (AnyMDx) for species-specific molecular detection (P. falciparum and P. vivax) of malaria in field settings. In our previous work, we have successfully explored a singleplex P. falciparum-specific AnyMDx system. The multiplexed AnyMDx system described in this abstract aims to further address the need for sensitive and species-specific detection of malaria in the field clinics. The multiplexed diagnosis system incorporates a ready-to-use reagent compact disk (with multiple independent species-specific reaction units) and a low-power, portable analyzer. Using whole blood as a testing sample, the multiplexed AnyMDx can deliver fast (40 mins from raw sample to answer), sensitive (∼1.6 parasite/μL), and specific (P. falciparum and P. vivax) molecular answers without any laboratory infrastructures.

BIOENIGMA: High Throughput Screening for Protein Based Materials

M. Demirel

Recent advances in the nanotechnology of materials, combined with parallel improvements in biotechnology and synthetic biology, have demonstrated that more complex biomimetic materials with properties engineered precisely to optimize performance can be achieved. Specifically, proteins provide unique advantages as advanced materials. For example, proteins can often self-assemble and form network materials with extraordinary properties such as extremely high durability or elasticity. More importantly, protein can evolve to new functionalities by gene mutations or duplications, which is a unique advantage compared to inorganic materials. Recently, we reported the development of a new technique to screen protein evolution based on laser-probing spectroscopy with sub-picosecond resolution. Our results demonstrate, for the first time, relative quantification of protein network topology in real time for directed evolution. Hence, using protein-based assembly and high-throughput screening, we could answer many fundamental questions in materials research, such as the fundamental long-range order in soft matter as well as developing new tools for advanced materials assembly. We are building a large library of polypeptides in bacteria as well as optimization using computational screening tools in order to
analyze how small changes in the protein sequence can alter protein-based materials properties. Our ultimate goal is to be able to tailor protein properties to fabricate desired biomaterials. Programming physical properties through directed evolution introduces a new design rule for the understanding of materials design.

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Mechanotargeting: Changes in Cell Shape Modulate the Overall Rate of Nanoparticle Endocytosis
P. Fattahi, Y.-T. Yeh, S.-Y. Zhang, S. Zhang, J. L. Brown, P. J. Butler

Changes in cellular morphology alter stress fiber alignment, which changes membrane bending and tension energies. All these changes eventually will affect the overall cellular nanoparticle uptake. To fully understand the changes in endocytosis process as a result of cell-shape alteration, we explored nanoparticle selectivity for endothelial cell in both single and monolayer orders. We utilized micro-printing of extracellular matrix proteins for single-cell engineering and home-built 3D near-field electrospinning (3DNFES) printer to create an aligned monolayer cell layer. Using these models, we showed that nanoparticles endocytosis in cells is inhibited when cells convert from a low-stress state (elliptical form) to a high-stress state (highly elongated) independent of cellular area and time. On the basis of these findings, we suggest optimal nanoparticle uptake to the cells can also be regulated by cellular shape and morphology, therefore providing a more effective disease diagnosis and targeting approach.

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Citrate-based Biomaterials for Drug Delivery and Tissue Engineering
G. Bora Kim, J. Yang

In recent years, citrate-based biomaterials have become an intense focus of research in the search for new functional biomaterials for solving pressing medical problems. Citric acid, a historically known intermediate in the Krebs cycle, is a multifunctional, nontoxic, readily available, and inexpensive cornerstone monomer used in designing our citrate-based biomaterials. In addition to the convenient citrate chemistry for the syntheses of a number of versatile polymers that may be elastomeric or mechanically strong and tough, injectable and photocrosslinkable, fluorescent and MR imaging-able, and/or tissue adhesive, citric acid also presents inherent anti-bacterial and anti-clotting characteristics, which make citrate-based biomaterials ideal for a number of medical applications. Furthermore, more recent studies have revealed the intriguing biological links of citrate to tissue regeneration, especially to bone regeneration. All these features make citrate-based biomaterials as the material of choice for many applications in regenerative medicine that are worth further developing. Herein, methodologies for the design and biomedical applications of citrate biomaterials will be discussed. Specific examples to be showcased include vascular grafts, bone implants, nerve guides, micro/nano-composites for orthopedic devices, bioinspired adhesives for wound healing, materials/cells/tissue for bioimaging, immune cell-mediated cancer drug delivery systems, and chloride sensor for cystic fibrosis diagnosis.

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Synthesis and Self-assembly of PNBE-PEO Amphiphilic Block Copolymer
C. Lang, J. LaNasa, M. Kumar, R. J. Hickey

Block copolymers are becoming universally used in biomedical applications. They have been used as drug carriers, prosthetic materials, tissue engineering substrates, medical membranes, and other biomedical materials. In this study, we have developed a new class of amphiphilic diblock copolymers combining two different living polymerization methods: ROMP (ring-opening metathesis polymerization) and anionic polymerization. Using this newly developed synthetic strategy, we were able to produce poly(norbornene)-block-poly(ethylene oxide) (PNBE-PEO) block copolymers with precisely controlled molecular weight and polymer block fractions of diblock and triblock copolymers which is crucial for self-
assembling desired colloidal nanostructures. We found that these polymers undergo self-assembly in water to form a range of nanostructures, which may be further used in applications related to drug delivery, templated synthesis, or membrane separations.

The High Field Magnetic Resonance Imaging (MRI) Facility fabricates its own MRI Radio Frequency (RF) resonators. These resonators are antennas that are used to transmit and receive electromagnetic signals to create MRI images. The optimal design and usage of RF coils is one of the keys to acquire high quality MRI images. The recent trend in using higher field MRI in order to create higher Signal to Noise Ratio (SNR) requires the fabrication of higher frequency antennas that match the operating frequency. However, the fabrication of RF antennas becomes more difficult at higher fields due to increased radiation loss and shorter wavelengths. A birdcage coil, one of the most commonly used homogeneous coils in clinical set ups at 1.5 T, 3 T, and 7 T, in high pass configuration was designed, simulated, and fabricated in this work to image stroke in a mouse model at 14.1 tesla field strength.

Phosphoserine (Pser), the phosphorylated amino acid highly abundant in Non-collagenous proteins (NCPs), and small molecules such as citrate are both integral parts of bone matrix and play important regulatory roles at the organic/inorganic interface for controlled bone cell activity and mineralization. Therefore, to better mimic the native bone, we incorporated Pser into citrate-presenting polymers to develop a new biomimetic biodegradable photoluminescent polymer, BPLP-Pser via a convenient polycondensation reaction. BPLP-Pser showed excellent photoluminescence properties, such as tunable emission and excellent photostability. Fluorescent imaging and analysis of BPLP-Pser films enabled the in vitro tracking of film degradation. Moreover, the incorporated Pser was found to facilitate the mineral deposition on polymer films, further improve its cytocompatibility, and even enhance the osteogenic activity of hMSCs on films evidenced by elevated alkaline phosphatase (ALP) production and increased gene expression of osteopontin (OPN). On the other hand, solute citrate and Pser that could be released from BPLP-Pser films, revealed their osteopromotive effect in terms of maintaining ALP production even at late stage and elevating OPN expression. Furthermore, BPLP-Pser/hydroxylapatite (HA) composite Microparticulate scaffold (Mps) system was developed. The Mps with high surface area greatly supported cell adhesion, and promoted the proliferation and osteogenic activity of hMSCs after packed into in vitro 3D culture models providing interconnective 3D porous structure, which led to the generation of intact and fluorescent cell-Mps constructs with defined shape and mechanical properties. Homogenous cell distribution was observed within the cell-Mps constructs, which is accompanied with massive production of extracellular matrix forming interwoven networks to bridge different Mps. In a rat femoral condyle defect model, the implanted BPLP-Pser/HA Mps presented their excellent osteoconductivity by providing an interconnective 3D framework allowing successful tissue ingrowth around the implants and throughout the defect, which led to extensive more peri-implant bone formation and significantly increased bone mineral density (BMD). H&E and Masson's trichrome staining further
confined the earlier bone formation and the facilitated bone maturation conducting along the BPLP-PSer/HA surface, suggesting its potential as a promising scaffold in orthopedic applications for speedy bone healing without the need for exogenous growth factors.

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A New In Situ Method to Measure Membrane Elasticity in Cell Membranes Using Fluorescence Lifetime Distribution of Dil
S. Son, H. S. Muddana, P. J. Butler

The elasticity of membranes governs membrane-dependent processes of protein activation, cell migration, mitosis, and other important cellular biological phenomena. Elasticity is described by membrane moduli, which represent the proportionality between stress and areal/flexural strain. Here, we demonstrate that the fluorescence lifetime of 1’-dioctadecyl-3,3,3′,3′-tetramethylindocarbocyanine perchlorate (Dil), which resides in the membrane, can be converted to membrane area-per-lipid (APL) and the values were directly used to determine elastic moduli of lipid membranes. Fluorescence lifetime of Dil was measured under confocal optics using time-correlated single photon counting. Fluorescence lifetimes (\(\tau\)), were converted to APL using the equations:

\[
A_L = A_o + A_f = A_o + \frac{x A_o}{\ln(K_{nr})-\ln(K_{mb})}, \quad \text{and} \quad \ln(K_{nr}) = -1.0476 * \ln(\tau) - 0.095,
\]

where \(A_o\) is the hardcore Van der Waals area (0.42 nm\(^2\)), \(A_f\) is free area, \(K\) is the radiative decay rate, \(K_{nr}\) is the non-radiative decay rate in low viscosity and \(x\) is a constant determined in control experiments. The mean and variance of APL applied to calculate compressibility modulus and bending modulus. Nanoliposomes were made via extrusion from lipid/dye mixtures of 1 mg/ml of lipid and 0.04 mole % Dil (diameters in the range of 100 to 150 nm) from both saturated and unsaturated lipids and the fluorescence lifetime of Dil embedded in nanoliposomes was measured. The Dil molecule decreases in lifetime in response to subtle increases in membrane APL resulting from temperature increases. In nanoliposomes with saturated lipids, both compressibility modulus and bending modulus have a linear relationship with head-to-head lipid thickness. Furthermore, we applied this assay to determine the membrane bending moduli in human cells. Results show that a newly developed method with lipophilic fluorescent probes, Dil, provides a way to measure APL and dynamic changes in APL to membrane compressibility and bending. Furthermore, this method is applicable to human cell membranes. Such results enable the measurement of the mechanical origins of cellular processes such as filapodia formation, and mechanical properties of nanoliposomes and membranous organelles for which there are currently no methods available.

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Mechanotargeting of Nanoparticles to Malignant Cells
Q. Wei, T.K. Zhao, P. Zhao, P. Butler, S.L. Zhang

Targeted delivery of nanoparticle (NP)-based diagnostic and therapeutic agents to malignant cells and tissues has exclusively relied on chemotargeting, wherein NPs are surface-coated with ligands that specifically bind to over-expressed receptors on malignant cells. Here we demonstrate that cellular uptake can also be biased to malignant cells based on altered cell mechanical properties, enabling mechanotargeting. In light of mechanotransduction, we direct the cell lines (HeLa and HCT-8) into different mechanical states and morphologies. In vitro delivery reveals that for non-metastatic cancerous cells the cell stress suppresses cellular uptake, counteracting with the exposed surface area of cells. Upon prolonged culture on stiff hydrogels, cohesive HCT-8 cell colonies undergo metastatic
phenotypic change and disperse into individual malignant cells. The dispersed cells are very soft and adopt an unspread 3D morphology, resulting in several-fold higher uptake than the pre-dispersed counterparts. Our study opens a new paradigm of harnessing mechanics for future nanomedicine.

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Towards a Real-time Data-driven Approach for Proactive Injury Prevention in Construction

J. Zhao, E. Obonyo

There is a need for more proactive injury prevention strategies that can enhance the progress towards zero injuries and fatalities in construction. This need is greater in chronic diseases such as Musculoskeletal Disorders (MSD). This paper presents preliminary findings from research directed at investigating the potential for leveraging an emerging sensor-based system to generate actionable data that can be used to improve the understanding of the contributing factors. One of the key barriers to injury prevention is the lack of reliable data on the complex interactions across contributing factors. Lessons can be learned from a "Web of Causation" approach that is being used to characterize and analyze the development progress of the disease. This is a data-intensive approach. It is the contention of this poster that the required data collection and processing needs can be addressed using emerging Wearable Technologies (WT). The main body of the poster outlines the pros and cons of existing systems. This is based on a comprehensive literature review of published work and experimental use of two low-cost WT. The discussion also proposes a strategy for designing and developing a WT application that can enhance construction injury prevention using real-time data.

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A Force-Threshold Criterion for Multicellular Epithelium Dispersion


Cancer metastasis is commonly regarded as a genetically programmed process. Yet recent studies have accumulated evidence that tumors may acquire metastatic ability through reciprocal interactions with their microenvironment. On the one hand, tumor progression is often accompanied with changes in tumor microenvironment, spanning from increased stiffness of extracellular matrix (ECM) to altered ECM composition and protein density. Reciprocally, cells sense biophysical cues from their surroundings, and respond by activating a cascade of biochemical signals that in turn regulate coordinated remodeling of cytoskeleton, cell-cell and cell-ECM adhesion junctions; all of which contribute to the progression of malignancy_ENREF_10. Despite increasingly accumulated evidence on microenvironment-induced malignant behaviors, no criterion exists for predicting the malignant transformation and tumor metastatic potential.

Cell migration, particularly the onset of cancer metastasis, involves dynamic generation and transmission of intracellular, intercellular, and extracellular forces. For cells in isolation, actomyosin contraction is transmitted to integrin-mediated focal adhesions, generating extracellular traction on the ECM. The traction reacts back to the cell, generating cell body stress. In multicellular microtissues, contractile forces are transmitted through both focal adhesions and cadherin-mediated adherens junctions, generating extracellular traction on the ECM on the one hand and long-range intercellular tension in the micro tissues on the other. Though it has been long conceived that stress homeostasis is essential to cell morphogenesis, survival, and normal functions, how mechanical force contributes to cancer metastasis and malignant transformation has remained elusive.
Herein we show that human colon carcinoma (HCT-8) cell colonies seeded on polyacrylamide (PAA) hydrogels undergo in vitro metastatic-like dispersion and malignant transformation in a gel-stiffness and colony-size dependent manner. To elucidate the role of cellular forces in this process, we measure extracellular traction and intercellular tension of the HCT-8 cell colonies at different stages of culture through traction force microscopy (TFM) and monolayer stress microscopy (MSM), respectively. A biophysical model is presented and used to generate cellular force landscapes in the parametric space of gel stiffness and colony size. The combined experimental and modeling analyses reveal a force-threshold criterion for the in vitro metastasis and malignant transformation, resembling the Griffith theory for crack propagation and material failure. Our finding underscores the potential importance of physical forces in directing phenotypic change of cells.

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Improving Energy Density and Power Performance of Li-Ion Capacitors Using Nano Graphite Anodes

A. R. Aref, C.-C. Chou, M. T. Lanagan, C. A. Randall, R. Rajagopalan

Electrochemical capacitors (ECs) are receiving extensive attention as potential energy storage device due to their high capacitance, rate capability, and long cycle life. The energy density of the capacitor is limited by the specific capacitance of high surface area double layer carbon cathodes, while the power performance is dependent upon the rate capability of the anode. In this investigation, we demonstrate that a high energy density lithium ion capacitor that can be charged and discharged between 2.2V – 4.2V with energy density exceeding 100 Wh/kg based on both the masses of the electrode and discharge time < 1 min can be fabricated. The capacitor was capable of being cycled at 1 A/g with 90% capacitance retention over 5000 cycles. The high voltage stability of the capacitor up to 4.2V was also determined using accelerated floating voltage tests. The high performance of the capacitor was due to the use of a high purity polymer derived carbon cathode with controlled pore size distribution along with a nanocrystalline prelithiated graphite as the anode.

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Scalable Manufacturing of Polymer Nanocomposites Using Oscillating Magnetic Fields

Y. Atescan, M. Spencer, S. Trivedi, M. Sharp, R. B. Branco, N. Yamamoto

Polymer nanocomposites provide advanced multifunctional, tailorable properties while retaining low density. However, bulk application is currently limited because fabrication of nanocomposites with precise control of nanofiller structuring and their interface conditions is currently missing. Active assembly using oscillating magnetic fields is a promising, scalable manufacturing method to organize nanofillers within polymer matrices in a non-contact and energy-efficient manner. Using magnetically-responsive nanoparticles, assembly can be achieved using small fields (~100s of G) in a short time (~15 mins). With oscillating fields, time-average negative inter-particle forces can be provided, improving tailoring of nanofiller structuring that is often dominated by innate positive inter-particle forces. In this study, first, magnetic assembly of nanofillers were parametrically studied for a model nanofiller: superparamagnetic iron oxide nanospheres (~15 nm diameter) in deionized water. Then nanofiller concentration and magnetic field properties (flux density, frequency, and waveform) were varied to tune the forces applied on the nanofillers (inter-particle magnetic forces, hydrodynamic forces, etc.) and their associated response time. From experimental observation, magnetic fields that oscillated in the low frequency range (< 1 Hz) were effective to tune inter-particle distances and thus interface conditions, balancing inter-particle magnetic attraction and particle diffusion. Second, the knowledge on
magnetic assembly obtained above is being applied to fabricate nano-structured magneto-active elastomers (MAEs) and nano-prepreg layers consisting of vertically aligned carbon nanotubes (CNTs). Ferromagnetic iron oxide nanoparticles were successfully assembled even in a highly viscous silicon rubber matrix. CNT nanofillers are being prepared by coating with nickel for magnetization and by surface treatment with diazonium treatment for improved suspension and dispersion within a thermoset matrix.

The production of laser modes is accomplished by confining gain within an optical resonator. This is conventionally accomplished through precise design and positioning of mirrors. Conversely, random lasers accomplish light confinement via random multiple scattering events. A suspension of TiO₂ nanowires in 2 mM rhodamine B dye solution is shown to support this phenomenon. Fluorescence produced by the excited dye is scattered by the particle matrix such that photons undergo a random walk within the gain region. A percentage of the resultant optical pathways take the form of closed-loops, resulting in laser buildup.

In suspension, the long axes of anisotropic particles are readily aligned by the application of an alternating current electric field. Simulation results predict that such collective alignment of TiO₂ wires can be utilized to change the scattering properties of a particle suspension dramatically due to anisotropic effects. Thus, reconfigurable wire alignment provides a means to tune the emission profile of a device between fluorescence and random lasing.

Optical metamaterials are a class of engineered materials which typically have unprecedented properties, like negative refractive index or optical cloaking capabilities. These properties are often facilitated by the rational design of sub-wavelength features of specific size, shape, and arrangement. For this reason, most experimentally realized metamaterials in the literature are made by top-down fabrication. As the demand for increasingly sophisticated devices continues to grow, it is important to develop metamaterials with dynamic functionality. While top-down fabrication allows for precise control over micro- and nanosized features, the resulting fabricated device typically is not reconfigurable. Hybrid top-down/bottom-up particle assembly is one possible way to achieve tunable and dynamic metamaterials. We demonstrate this by using electric fields, propagating from lithographically patterned co-planar microelectrodes, to drive particle assembly. Electric field driven assemblies are advantageous because they allow for assembly reconfigurability by toggling the field on/off and tunability by varying the electric field conditions. Here, we characterize the assembly behavior of metamaterial-relevant composite metal/dielectric particles made by templated electrodeposition of metal salts, subsequent glass coating, and finally selective metal etching. This process yields nanowires with stripes of gold separated by hollow solvent-filled etched regions, all encased in a silica shell. Therefore, smaller gold segments can be pre-ordered within a larger nanowire by synthesis prior to assembly, providing additional degrees of spatiotemporal control over the assembly. Additionally, we show that adjusting the striping pattern changes the
assembly behavior of the composite particles. Thus, assembly motifs of interest can be realized by *ad-hoc* particle design. Finally, we show a proof-of-concept reconfigurable polarizer as an application of assemblies of composite metal/dielectric particles.

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**Direct Laser Writing via Laser Induced Thermal Voxels**

C. Kindle, L. Zarzar

Ease of customization and fabrication are significant driving forces in the realm of materials innovation and production. We aim to develop a methodology for 3D integration of materials that marries solvothermal synthesis with laser patterning. By generating a femtoliter-scale solvothermal reaction volume at the focus of a laser (“laser induced thermal voxel” or LITV) with temperatures that can exceed 2000 K, we can confine and pattern chemical synthesis for a broad range of materials with high chemical tunability, including metals, oxides, and composite materials directly from solutions of the desired precursors. LITV implements a streamlined process in which an absorbing material converts the energy provided by a laser to thermal energy at the tightly focused volume, promoting the solvothermal synthesis of inorganic nanomaterials directly from a precursor solution. The synthesized nanoparticles are deposited directly at the liquid/solid interface and can be patterned or “drawn” by scanning the laser focus over the surface. The material deposited can be controlled by changing different aspects of the synthetic process such as solvent, pH, laser power, scan rate, concentration, and presence of surfactants.

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**CVD Growth of Graphene and hBN for 2D Heterostructures and Integration**

J. W. Kronz, R. Lavelle, J. Redwing, D. W. Snyder

Two-dimensional (2D) materials are paving the way for the next generation of nanoelectronics, offering unique electronic and mechanical properties in materials confined to a plane of atoms. Materials of current interest are graphene and hexagonal boron nitride (hBN). Both of these materials have attractive properties for electronic devices, but show superior properties when integrated together in a van der Waals (vdW) heterostructure. Reports have shown that graphene transferred onto a 2D hBN substrate can radically boost mobility. The mobility enhancement using hBN as a substrate can also be seen when MoS$_2$ is placed onto hBN, further demonstrating the usefulness of integrating 2D materials onto hBN.

Chemical vapor deposition (CVD) is a useful method to fabricate these structures as it allows for large area growths in addition to crystal structure and thickness control. By enabling the growth of 2D materials directly on top of one another, higher quality films and heterostructures can be created.

CVD of graphene is currently conducted growing on a copper foil substrate at low or atmospheric pressure and high temperature followed by transfer to a more suitable substrate. This approach typically results in a monolayer of high quality graphene. The transfer process is a wet transfer process that requires a PMMA support layer on top of the graphene, while the copper is selectively etched off the back of the graphene.

Growth of hBN is carried out using a two-step process of a low temperature growth with a high temperature anneal. Growth occurs at low pressure using
borazine (B₃H₆N₃) as a source. Borazine is created by sublimating a borane ammonia complex (H₃N·BH₃) powder upstream from the substrates, which are either sapphire or (111) silicon. These growths yield a thin film that has a surface roughness of less than 0.2 nm, which is ideal for integrating with other 2D materials to enhance carrier mobility and optical properties.

This poster will discuss recent results for the growth and transfer of large-area graphene, the growth of high quality hBN film and the integration of these materials, and illustrate the benefits of hBN substrates for integration of various 2D materials including graphene, MoS₂, and WSe₂.

Block copolymers are linear chains composed of chemically distinct polymer blocks that are connected through covalent bonds. Due to thermodynamics of mixing, block copolymers self-assemble into nanoscale morphologies that minimize interfacial surface area between unlike chain regions. The following research aims to develop functional materials by hierarchically organizing inorganic nanoparticles using the self-assembly of block copolymers under the constraint of immobilizing one of the chain ends to inorganic nanoparticles. Here we have developed an approach for controlling the polymer grafting density and molecular weight using a “graft-from” polymerization approach. We have focused our synthetic work on polymerizing poly(norbornene)-block-poly(ethylene oxide) block copolymers from the surface of silica nanoparticles. The precise chemical control of the block copolymer architecture allows us to study the fundamentals driving nanoscale self-assembly. Hybrid polymer/inorganic composites could provide a novel mechanism of ordering inorganic material within soft matter, with resulting materials possessing enhanced mechanical, thermal, and optical properties.

Integration of materials into miniaturized electronic devices requires understanding their properties at reduced length scales and dimensions, which are often different than their bulk counterparts. Such understanding, which often correlates with factors including stoichiometry, dopants, crystallographic defects, and strain, can be further utilized to modulate the properties of the nanomaterials. Here we present the modulation of the metal-insulator transition (MIT) temperature in nanoscale vanadium dioxide (VO₂), which, in bulk, undergoes a reversible phase transition between a high temperature metallic phase and room temperature insulating phase with a transition temperature of 68°C. With the microscopic, crystallography, and thermal analysis capabilities at Penn State’s Materials Characterization Lab (MCL), we were able to investigate the influence of size and interfacial strain on the MIT temperature in solution-synthesized epitaxial VO₂-TiO₂-VO₂ nanoscale heterostructures. We found that the synthetic protocol impacts the domain and interfacial characteristics of the VO₂-TiO₂-VO₂ nanostructures, which is useful knowledge that can be applied to other applications of VO₂ nanomaterials, including memory devices, Mott transistors, metamaterials, and gas sensors.
Condensation and Fog Harvesting on Bioinspired Slippery Rough Surfaces

X. Dai, N. Sun, B.B. Stogin, J. Wang, L. Wang, T.-S. Wong

Droplet nucleation and repellency on surfaces are two fundamental issues that are critical to condensation heat transfer. State-of-the-art liquid-repellent surfaces cannot achieve exceptional droplet nucleation and repellency concurrently due to the unfavorable hydrophobic surface chemistry and droplet pinning on surface defects. While hydrophilic surface chemistry favors droplet nucleation, hydrophilic surfaces with excellent droplet nucleation and removal capabilities have not been reported. Inspired by the unique functions of pitcher plants, and lotus and rice leaves, we present a hydrophilic directional slippery rough surface (SRS) that is capable of rapidly nucleating on the hydrophilic functional groups and removing water droplets on the super slippery water-lubricant interface. Our surfaces consist of nanostructured microchannels with infused hydrophilic liquid lubricant into the nanotextures alone. We have demonstrated that the SRS, owing to its large surface area, hydrophilic slippery interface and directional droplet mobility, significantly outperforms state-of-the-art hydrophobic liquid-repellent surfaces including superhydrophobic surfaces and slippery liquid-infused porous surfaces in condensation and fog harvesting applications.

Band Filling and Electric Field Effects on Anisotropic Magnetotransport of Two-dimensional Electron Gases at SrTiO$_3$ (111)-, (110)-, and (001)-oriented Surfaces

L. Miao, J. Wang, R. Du, Y. Yin, Q. Li

Two-dimensional electron gases (2DEGs) at the interfaces or surfaces of band insulating SrTiO$_3$ (STO) have been a fertile platform for a host of emergent phenomena such as quantum Hall effects, superconductivity, and ferromagnetism. They are also an important basis for realizing oxide electronics. These properties are largely governed by the structures of Ti 3d band as well as Rashba spin-orbit coupling at the surfaces or interfaces. One example is the anisotropic magnetoresistance (AMR). Unlike magnetization-induced AMR in magnetic systems, AMR in non-magnetic systems reveals other subtle physics. However, AMR in STO 2DEGs has not been fully understood yet. In this poster, we report a systematic study of AMR of STO surface 2DEGs on two sets of 2DEG states: one with different carrier densities, without a gating electric field, and the other with a nearly constant carrier density, but with different gating electric fields. These states allow us to separately study the effect of band filling and the effect of the electric field on AMRs. To our surprise, AMRs of (111)-, (110)-, and (001)-oriented 2DEGs exhibit dramatically different responses to the tuning of band filling, and perfectly match with the symmetries of the gate-selected bands, revealing a close relationship between AMR and the band structures. On the other hand, AMRs of 2DEGs with various orientations show similar responses to electric field tuning, verifying that they also rely on Rashba effect. These results not only provide understandings toward the origins of AMR, but also open a new route to probe the band structures via transport characterization of electron gas systems.

Advanced Multifunctional Energy Materials and Systems

Q. M. Zhang, T. Zhang, Y. Thakur, H. Xi, M. Lu, Xin Chen, Y. Zhou, Y. Hou, Q. X. Yang

This poster will present recent advances in the Laboratory for Advanced Multifunctional Energy Materials and Systems in the area of nanocomposite polymer dielectric capacitors with high dielectric constant, low loss, and high operating temperature, nanocomposites ionic system for energy harvesting with high energy density, electrocaloric polymers and ceramics and their related devices, and ultrasensitive biomagnetic sensors.
Ultra-thin layered materials exhibit unique properties such as physical flexibility, chemical inertness, and thickness dependent optoelectronic characteristics, making them versatile for a wide variety of applications. The Robinson group at Penn State focuses on better understanding the growth and electronic properties of a variety of 2D materials, ranging from better-known materials such as graphene or MoS₂ to novel 2D materials such as GaN. This poster provides an overview of the research topics done by the group, including: metal organic chemical vapor deposition of TMD selenides and expansion to wafer scale single crystal growth; oxide vaporization synthesis of MoS₂ on various substrates; Mott transition characteristics of TaS₂ as a function of substrate; direct growth of and electronic transport across vertical and lateral 2D heterostructures; growth and band alignment tuning of epitaxial graphene; growth, discovery, and characterization of novel 2D selenides and III-V materials; and other work furthering the field of 2D electronic materials.

Metamaterials are a class of man-made materials which showcase unnatural dielectric and optical behaviors, such as negative permittivity and refraction. By integrating a controllable plasma array into the metamaterial, electromagnetic properties can be dynamically altered. This integration is possible due to the resonant nature of metamaterials, which creates strong electric fields that can break down the surrounding gas to ignite plasma. To evaluate constituent material performance for plasma production, we use split-ring resonators to compare different metals, and now we have developed a double-ridge waveguide (DRWG) to measure the performance of resonating dielectric blocks. DRWGs focus electric field between conductive ridges which run along the top and bottom of the waveguide, and a dielectric block is placed between the ridges. The DRWG is then vacuum-pumped and backfilled with low-pressure argon gas and, when powered, forms argon plasma within a gap between the dielectric and upper ridge. Simulations show that the dielectric block sharply increases the electric field strength within the gap, enabling this plasma ignition. Argon pressure is varied to collect Paschen-like data and determine minimum power needed for plasma ignition. In this setting, dielectric work functions and the electronic properties of plasma can be closely measured.

The Magneto-Active Structures and Composites Lab (MACS) fabricates and models magnetically active materials for origami, locomotive, and sensory applications. Current projects within the lab include the fabrication and characterization of hard magnetic materials, the development of a multi-material printer capable of printing magnetic material, as well as the mathematical modeling of multi-field structures.

For origami applications, magneto-active elastomers (MAE) are fabricated by embedding hard magnetic particles within an elastomer matrix. As an MAE cures, an external magnetic field can be applied to align the particles in a specified orientation, such as an in-plane alignment or an out of plane alignment. MAEs can then be strategically placed on flexible material, to replicate known origami structures. MAEs have a preferred magnetic direction. When this preferred
magnetization is not parallel to an applied external field, torque will be generated, and the MAE will rotate to align with the external field.

To calculate the torque generated by an MAE, the remanent magnetization of the MAE must be determined. To find the remanent magnetization, a vibrating sample magnetometer (VSM) is used. The VSM applies an external magnetic field on the MAE, and measure the magnetic moment produced. Using the resulting hysteresis loop, the magnetic properties of the MAE can be determined.

Complementary to the experimental side of the MACS Lab, is the modeling side. Using Comsol Multiphysics and in-house code, magnetically active material and electrically active material are modeled and compared to experimental data.

56 FAST Manufacturing of Advanced Nano-/micro-structured Metallic and Ceramic Composites


Field assisted sintering technology (FAST) is a potential solution to bulk fabrication and joining of nano-/micro-structured metal and ceramic composites. Unlike the conventional sintering and hot pressing processes, in the FAST set-up, the powders, pressed inside a die, are applied with radiant heating from the graphite mold and Joule heating from the DC current flown through powders. With the effective combination of pressure, temperature, and localized heating at the grain boundaries, the FAST requires reduced sintering time (down to a few minutes) and temperature, and thus can provide small-grained composites. In our collaborative work, engineering of two materials are explored using FAST: joined interfaces of nickel (Ni)-based superalloys and nanoporous ceramic composites.

First, we study to engineer Ni-based superalloy interfaces using FAST. To provide high strength and creep resistance at extreme temperatures (~1400 °C), turbine engine blades currently consist of mechanically joined single crystalline and polycrystalline Ni-based superalloys. To eliminate the heavy mechanical joint and thus to increase performance, methods to bond these dissimilar materials need to be investigated. Unlike linear friction welding that introduces thick and non-homogenous interfaces, the FAST can potentially provide clean, nano-grained interfaces to effectively distribute mechanical and thermal stresses. The effect of FAST sintering parameters and the mixtures of powders (Inconel 625 micro powders of ~44-105 µm, SiC and TiC nanoparticles of ~80-100 nm and ~40-60 nm) are studied on morphology (grain size and phase) and mechanical properties (stiffness, hardness, including at high temperatures).

Second, we study to manufacture nano-porous boron carbide composites using FAST to induce quasi-ductile deformations and thus to potentially improve fracture toughness. With high strength, low density, corrosion resistance and thermal stability, ceramics are suitable for extreme aerospace environment, but their applications are currently limited due to low fracture toughness. Our recent nanoindentation studies on anodic aluminum oxide (AAO) samples have shown that nanoporosity can introduce quasi-ductile deformations; highly localized shear-banding-like nanopore deformation and other non-brittle deformations are promoted by increased free volumes and grain boundary effects. The combination of sample parameters (interpore distance, porosity, and phase) of nanoporous AAO membranes were identified to trigger such quasi-ductile deformation. Based
on this knowledge, boron carbide ceramic composites will be FAST-sintered to yield small porosity, grain sizes, and grain boundaries. Powders of different size and of high property contrast (boron carbide powders of ~0.6-1.2 μm, titanium oxide of ~40 nm, and carbon black nanopowders of ~42 nm) will be sintered. Multi-scale characterization will be conducted on these samples, in relation to their micro-structures.

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Ceramic Coating for Corrosion (C3) Resistance of Nuclear Fuel Cladding


The Fukushima-Daiichi accident motivated research for accident tolerant fuels that are more forgiving in the case of a loss-of-coolant-accident (LOCA). The aim of this research was to develop ceramic coatings for zirconium based nuclear fuel cladding that are corrosion resistant and can withstand normal operation and accident conditions. Single layer TiN, single layer Ti$_{1-x}$Al$_x$N and multilayer TiN/Ti$_{1-x}$Al$_x$N coatings were deposited on flat and tubular ZIRLO® substrates by using cathodic arc physical vapor deposition (CA-PVD). Such coatings have been widely used for years on high-speed tool steels, cemented carbides, and cermet substrates for various cutting and finishing operations in the tooling industry since they provide enhanced hardness, wear resistance, and chemical inertness. Autoclave corrosion tests of the coated materials were performed in static pure water at 360°C and 18.7 MPa at Westinghouse Co. (Pittsburgh, PA) for up to 128 days. Following the autoclave test, weight gain analysis was used to characterize corrosion performance of the coated materials. Several characterization methods were used to examine the materials before and after the corrosion test including scanning electron microscopy (SEM) for morphology examination, energy dispersive spectroscopy (EDS) for elemental analysis, and X-Ray diffraction (XRD) to determine phases present. Coating adhesion and corrosion performance was systematically improved through the optimization of parameters involving substrate surface preparation method, substrate surface roughness, titanium bond coating thickness, coating thickness, deposition parameters, and multilayer design architecture. We determined deposition parameter effects on coating morphology, composition and adhesion property; identified optimized cathodic arc physical vapor deposition parameters to enhance adhesion of the coatings on flat and tubular ZIRLO®; determined corrosion behavior of TiN and TiAlN in nuclear reactor environment. The results indicated that the corrosion performance was substantially improved for the multilayer design considering an order of lower weight gain than the uncoated ZIRLO® without spallation. We conclude that monolithic TiN, monolithic TiAlN, and multilayer TiN/TiAlN coatings are applicable on ZIRLO® substrates by using the cathodic arc physical vapor deposition method and optimized multilayer TiN/TiAlN coatings on ZIRLO® enhance corrosion resistance at normal operation and extreme environment conditions.
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Manufacturing and Uniformity of Grain Textured Piezoelectric Ceramics
For many decades, metals and polymers benefitted from the ability to enhance electrical and mechanical performance by creating highly directional microstructures via rolling, drawing, directional cooling, or other similar processing techniques. Directional tailoring of performance for oxide materials has been largely limited to taking advantage of anisotropies in single crystal materials. Meanwhile, traditional technical ceramics remain unimproved with respect to commercialized products. This poster outlines the process technology and scale up considerations for tailoring asymmetric, directionally oriented ceramic microstructures, with a focus on achieving near single crystal performance from highly oriented ceramic piezoelectric materials. The key principle exploited is the ability of highly anisotropic grains to be added to and then aligned inside a ceramic green body such that they seed pronounced asymmetric grain growth. Critical processes, including template synthesis, template alignment via tape casting, part fabrication, process controls, and process characterization, will be discussed. The engineering challenges associated with scaling each process step and related factors critical to economically feasible manufacturing will be outlined.

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Cold Sintering: An Extremely Low Temperature Processing Route for Ceramics and Related Composites
J. Guo, M. Sengul, X. Zhao, K. Tsuji, B. Li, W. Chen, A. Baker, M. T. Lanagan, C. A. Randall
The conventional thermal sintering process of ceramics is generally performed at high temperatures, typically ranging from several hundred to tens of hundreds of degrees Celsius, to enable the mass transport processes that allow the atoms, cations, or molecular groups to diffuse across the boundaries of adjoining particulates. Cold sintering process (CSP) is a new sintering technique that we are exploring to sinter ceramics and ceramic-based composites with the assist of a transient liquid phase, such as water and acids. With CSP, the sintering temperatures of ceramics can be decreased from several hundreds of degrees or even tens of hundreds of degrees to lower than 300 °C. Cold sintering has been successfully demonstrated for a large number of chemistries (oxides, carbonates, bromides, fluorides, chlorides, and phosphates) and a diverse range of applications, including ferroelectrics, microwave dielectrics, semiconductors, Li-ion batteries, and thermoelectrics. In addition, the low sintering temperatures enable the co-sintering of new types of ceramic-polymer composites. Several ceramics and related composites with different applications are selected to show the overall diversity of CSP and the preliminary simulation result is also included to discuss the mechanisms of cold sintering.

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Additive Manufacturing: An Enabling Technology for Design Optimization
B. Hanks, M. Frecker, M. Moyer
Additive Manufacturing (AM) presents a unique opportunity for design optimization and customization, where optimized designs are not necessarily manufacturable with traditional processes. We demonstrate the ability of AM to allow greater freedom for design optimization with two cases: an endoscopic surgical tool and impact absorption cellular arrays.

In the case of radiofrequency ablation treatment, the shape of the tool determines the shape of the treatment and ultimately its efficacy. Using a genetic algorithm to optimize the shape of tool, we have shown an increase in treatment efficiency from 25% to 71% for a 2.5cm spherical treatment zone. With the use of AM, these custom and optimized surgical tools may become a reality.
Lattice, or cellular, structures are readily manufactured through AM processes. Compliant cellular structures allow for varied directional stiffness and energy absorption during impact. Previous work has shown that design optimization can be used to manipulate a unit cell’s topology and optimize it for impact absorption at specific velocities. While the initial cells were 2D, metal AM allows for manufacturing of complex 3D cells that can be used to tailor mechanical properties in various directions. The ability to adapt a structure’s stiffness properties shows unique opportunities in orthopedics and energy absorption by removing many of the manufacturing constraints that would typically be associated with these complex structures.

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**Effect of Alloying Elements (Cr and Al) in Nickel-based Alloys in Molten Sulfate Environments**

K. Kumar, H. Kim

Extreme thermal and chemical environments in gas turbines cause premature failure of turbine materials due to hot corrosion. Contaminants in the fuel during combustion are converted to molten salt deposits composed of low melting alkali halides and sulfates. This study will report the interfacial degradation reactions at the substrate/molten sulfate interface using electrochemical techniques of potential sweep, impedance spectroscopy, and cyclic voltammetry to elucidate the impact of alloying elements in controlling the degradation reactions at 700 °C. This study was guided by the hypothesis that the interfacial degradation behavior is dictated by electrochemical reactions due to the dissociation tendency of molten sulfates (Na$_2$SO$_4$ → Na$^{2+}$ + SO$_4^{2-}$). The electrochemical corrosion properties will be correlated with exposure tests by characterizing corrosion products using SEM/EDS, XRD, and thermal analysis. Both the electrochemical and exposure tests were conducted in eutectic LiCl-KCl with the addition of 10mol% Na$_2$SO$_4$ under reactive gaseous atmosphere (O$_2$-0.1%SO$_2$).

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**Additive Manufacturing Shape Memory Alloys: Heat Treating to Tune Microstructure**

B. A. Bimber, R. F. Hamilton, T. A. Palmer

Additive manufacturing (AM) shape memory alloys (SMAs) affords the materials engineer a tool to tailor material behavior for practical applications by tuning microstructure with respect to composition, grain structure, and microconstituent phase morphology. The AM microstructure dictates the underlying martensitic phase transformation (MT) that begets shape memory behavior. The ability to tune the microstructure with AM can expand integration of SMAs into new application spaces. AM is a layer by layer deposition process. For this work the laser directed energy deposition (LDED) AM technique is employed. Powder flows into a molten pool that follows a prescribed build plan/path. Consequently, melting/remelting, solidification and reheating are inherently localized. Binary NiTi is the work horse commercialized composition. Though AM of NiTi alloys has been the subject of many works recently, correlations between the AM process and the different microstructural length scales of the AM material microstructure (i.e. composition, grains, and microconstituents) are not well understood. Solution and aging heat treatments were employed to alter the material microstructure post-deposition. Aging is well-known to precipitate Ni$_4$Ti$_3$, which is beneficial in promoting strain recovery, from 3 up to 8 times that of typical liner elasticity, after unloading at constant temperature, which is referred to as superelasticity (SE). In-situ and full-field strain analyses resolved the evolution of fine scale strain measurements throughout load and unload deformation. With this, this work provides
unparalleled insights into the consequences of the interactions of the MT and the microstructures resulting from AM. The results show that post-deposition heat treatments consisting of solution treating followed by aging can be beneficial for improving multi-scale strain recovery, and the accompanying MT can mimic conventionally processed alloys.

This poster highlights the study of Vertical Bridgman (VB) growth of topological insulators (TI’s) Bi$_2$Se$_3$, Bi$_2$Te$_3$, and Bi$_2$Te$_x$Se$_{1-x}$. These materials are of interest to the materials science and physics community because they are bulk insulators with conducting surface states protected by time-reversal symmetry.

In particular, this study examined the effect of varying the stoichiometric composition of the binary and ternary constituents and other process-related variables that may introduce impurities into the crystal structure.

Additionally, this poster will discuss our ampoule preparation process and VB growth conditions. Specifically, the ampoule coating was introduced as a process variable in this study. We also sourced materials with different purity levels to examine the effect on the TI’s.

After growth, the TI boules were imaged and exfoliated for characterization. The mobility, carrier concentration, and resistivity of the materials were characterized by Hall Effect measurements conducted at varying temperature levels. Energy Dispersive Spectroscopy (EDS) was used to analyse the constituent ratio as a function of boule length. Glow Discharge Mass Spectrometry (GDMS) was used to quantify the impurities in the TI’s grown with different source material purities and ampoule coatings.

Of particular interest was the effort to grow high quality TI’s with low impurity levels and low bulk carrier concentrations. We will present our findings for different material compositions investigated in this study.

This work was conducted as part of the bulk growth initiative of the 2DCC/Materials Innovation Platform (MIP) at Penn State, in conjunction with the Applied Research Laboratory (ARL).

The influence of γ-quinacridone as a β-crystal nucleating agent in injection molded isotactic polypropylene (iPP) is discussed. To improve the understanding of iPP crystal polymorph development, the molding process was first simulated to establish shear and cooling rate profiles at specific locations within the part. Physical samples were injection molded and characterized via polarized-light optical microscopy (POM) and X-ray diffraction (XRD). The XRD analysis of these samples showed that in the highly nucleated system (500 ppm), the only region that was unable to produce the β-structure was at the skin layer. The cooling rate associated with the quench at the mold wall was estimated to be greater than 600 °C/s using simulation; confirming previous studies that β-growth is not supported at that cooling rate. The non-nucleated sample did not produce β-crystals at any cooling rate in the quiescent condition. With the addition of
shear and pressure in this process, the sample formed β-crystals at 100-300 µm from the skin and in to the core. Interestingly, the mold filling simulation did not predict shear in the core. The β-crystals formed in the core are attributed to shear effects in the injection unit of the molding machine that were not modeled in this simulation, nor would be typically modeled in any analysis. This “melt-memory” effect has shown to be significant in these molded samples, as such history can change the expected crystal polymorph and resultant bulk material properties. Mechanical analysis of the materials showed that greater nucleation content, and, therefore, higher content of β-crystals as well as spherulite size reduction increased the ductility of the material. By better understanding the processing conditions that produce the specific material polymorphs, the final part properties can be better predicted before manufacturing.

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Graded Glass-ceramic Interface

S. Nazarian, C. Pantano, P. Colombo, M. Marangoni, M. Hojati, H. Ye

This poster presents innovative material interfaces, achieving seamless and/or sequential transition from ceramized geopolymer cement to transparent glass, executing the concept of seamless architecture by sintering or casting techniques, making possible novel sustainable practices in production processes and in building’s performance (i.e.: less embodied and operational energy). This technology presents novel solutions for building in harsh weather where impermeability between and through surface materials is required; highlighting unique advantages of additive manufacturing in the design and production of functionally graded materials, and seamless architecture.

Our approach has many potential applications in the arts, industrial design, and architecture, permitting lower embodied and operating energy, construction details never imagined before, and surface conditions exhibiting multiple optical and structural characteristics. Imagine for example, transparent windows within opaque walls while achieving structural, thermal, optical, and even a graded transition between glass and opaque materials such as geopolymer concrete and advanced closed porosity ceramics. We have used casting and kiln forming processes to fabricate our prototypes and have already achieved strong bonds between glass and geopolymer cement and also glass-foam. Several formulations of Geopolymer (GP) based ceramics and Glass-Foam (GF) based ceramics were seamlessly interfaced with glass creating the desired structural and optical continuity, resulting in airtight and watertight transition between the materials without any mechanical joints or connective tissue. Our vision is to expand this technology to engage 3D manufacturing and other free-form fabrication technologies.

Generative concept: In contemporary architecture, when different building parts or materials meet an overwhelming variety of joints are present. These joints address air-tightness, water-tightness, load bearing, thermal insulation, or multiple other issues that occur where buildings parts or materials meet. We find joints between components or materials on the same wall, such as window frames, exterior finishing, thermal insulation layers, and load-bearing concrete blocks.
Conventionally, a joint between two materials or components is resolved by introducing a third material/component that either chemically or mechanically fastens them. For example, a metal frame is typically used to mechanically fasten glass inside a masonry wall. This type of mechanical joint requires an array of smaller joints to deal with a number of functional requirements to create the necessary thermal, fluid, vapor, and acoustical barriers and insulating layers, each introducing additional complexity, involving numerous building trades, and adding material and labor costs.

As a result, coordination between various trades is complicated and difficult, there are more potential points of failure, and the security of the seal over time cannot be guaranteed. It is important to rethink these conventions. This research makes possible impermeable seams and/or seamless interface(s) between building materials and components to address functional, optical, and structural requirements for applications in the building construction, arts, industrial design, aerospace research, and architecture.

The poster exhibits the interconnectedness of three main paths of exploration that the award-winning multidisciplinary team of faculty, staff, and students of PSU pursued in NASA's 3D-Printed Habitat Challenge. These included the development of novel concrete formulations, development of autonomous 3D printing processes, and design and development of the overall 3D printing system necessary to print large structures. The main goal of the project was to advance the additive construction technology needed to create sustainable housing on earth and for deep space exploration.

In addition, the poster reveals the relevance of the teams' choices to the significant and pressing issues of global warming and exhibits that the building industry which now has a huge carbon foot-print, can make a measurable contribution to reverse that trend by engaging in sustainable practices in the design and production of materials and construction techniques and processes. The project’s aim was to develop additive manufacturing technology to 3D print habitats that can withstand harsh conditions using a specially formulated concrete made from recycled and indigenous materials that can be found locally on Mars, but can be applicable on Earth.

The production of the geopolymer binder(s) used in the formulation of the concrete designed by the team does not emit carbon dioxide into the atmosphere, unlike the production of Portland cement (the most common type of cement). Current expertise in 3D printing, also called additive manufacturing, is leveraged to transfer expertise with smaller-scale printers and their associated processes to the large-scale printing of concrete.

The project was based on previous research aimed at developing functionally graded materials and verifying the possibility of designing and constructing seamless buildings, which can have a significant impact on architectural language and building processes.
The interdisciplinary team of Penn State researchers, included representatives from the departments of architecture and civil and environmental engineering, and the School of Engineering Design, Technology, and Professional Programs (SEDTAPP). To further develop the technology and assess its impact on architectural language and building processes, the first interdisciplinary design studio is being conducted this fall in the department of architecture, which makes use of our newly established "Concrete AM" lab.

Two different porous metal-organic frameworks (MOFs) Cu$_3$(btc)$_2$ (HKUST-1) (btc = benzene-1,3,5-tricarboxylic acid), Cr$_3$F(H$_2$O)$_2$O(bdc)$_3$ (bdc = benzene-1,4-dicarboxylic acid) (MIL-101) and their monolithic composites with silica aerogel were investigated for methane adsorption capacities for natural gas fuel storage in vehicles. Composites of MOF and silica aerogel were prepared to increase their methane uptake capacity on a volume basis by filling in the void space with aerogel while keeping the volume of the MOF and composite constant. The MOFs were prepared using solvothermal method, while their monolithic composites were synthesized by mixing the MOFs with aerogel solution which was prepared using methyltrimethoxysilane by acid-base catalyzed method. According to powder X-ray diffraction, the MOFs are pure and highly crystallized, and the aerogel composites maintained the original structure of the MOFs. Nitrogen adsorption-desorption isotherms at 77 K suggested the shape is characteristic of Type I which indicated that all the materials are microporous. Methane adsorption isotherms were measured at room temperature up to 35 bars. Among the four materials, Cu$_3$(btc)$_2$ aerogel composite showed the highest adsorption (9.8 wt.%) at room temperature although the capacity of Cu$_3$(btc)$_2$ itself is much lower (6.8 wt.%) than its composite with aerogel on a constant volume basis. However, it was found that there was only a small difference in methane adsorption capacities between Cr$_3$F(H$_2$O)$_2$O(bdc)$_3$ and its composite with aerogel, but further studies are in progress to determine the cause of this small difference.

Capacitive deionization (CDI) is an energy efficient and economical desalination technique. With the current water demand for irrigation and the need for the conservation of drinking water, capacitive desalination of brackish water offers an alternative way to reduce the tension between irrigation and the direct consumption of water. This research encompasses the full process cycle consisting of carbon production, activation, characterization, electrode fabrication, electrochemical testing and analyses for capacitive desalination rate, capacity, and cycling stability. The electrodes are fabricated using various carbon precursors including commercially available activated carbon cloth, polyfurfuryl alcohol (PFA) derived carbon and biomass-derived (coconut shell, switchgrass) high surface area activated carbon materials. The goal of the research is to compare the adsorption rates and capacities of these carbon materials as well as their charge and regeneration efficiencies in order to determine which of these activated carbon materials is best suitable for this technique. Our investigation showed that microporous coconut shell derived carbon had the best charge efficiency while polymer derived carbon had the highest adsorption rate. The pore size distribution of the carbon had a profound impact on CDI performance. Microporosity improves salt adsorption capacity. Macroporosity facilitates
transport, improving the adsorption dynamics, but at the cost of charge efficiency. Among the carbons tested, commercially available coconut char carbon, YP50 had the highest charge efficiency of ~ 60% and a salt removal capacity of ~5 mg/g. Salt removal capacity increased with applied voltage for all the carbons.

### 69
**Flow-induced Crystallization of Nylon 6/6**


When a semi-crystalline polymer melt is subjected to sufficiently intense flow before crystallization, the crystallization kinetics are accelerated and the crystal morphology is transformed from spherulites to anisotropic structures. The phenomena are called flow-induced crystallization (FIC). In this study, the FIC of Nylon 6/6 was investigated using rheology and polarized optical microscopy. For rheological investigation, small amplitude oscillatory shear (SAOS) tests were performed to monitor FIC kinetics. As a shearing work was imposed on a Nylon 6/6 melt at 270 °C from 10 to 10^7 Pa, the onset of crystallization at 245 °C was accelerated from 628 s to 26 s. For quantitative analysis for the acceleration, Avrami equation was used with Pogodina’s storage modulus normalization method. Based on the analysis, the degree of acceleration became greater after the transition of Avrami exponent from 3 to 2 at the imposed specific work of 10^5 Pa. Moreover, the shear-induced morphological transformation was observed using polarized optical microscopy. At nearly zero shear rate, large spherulites were observed without cylinderites, while a mixture of small spherulites and cylinderites was shown at a shear rate of 10 s⁻¹.

### 70
**Surface Chemistry of Glass and Tribology**

N.S. Sheth, J. Luo, X. He, H. Liu

Physisorbed molecules on solid surfaces often influence the surface chemistry and mechanical response of the solid surface. In the case of silicate glasses, it is believed that water can nucleate and expand strength-controlling defects on the glass surface, reducing its usable strength. Surface treatments, such as acid leaching and heat treatments, result in controlled alteration of the surface chemical structures (BO, NBO, OH), chemical reactivity and mechanical response. This allows for the evolution of surface structures and hydration sites to be identified and quantified spectroscopically. By combining information obtained from surface-sensitive spectroscopy techniques (SR-IR, ATR-IR, XPS, SFG) with the mechanical response to shear and normal loads, a relationship between the silicate glass surface chemistry and mechanical response can be deduced.

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**Exploring the Cause of Non-graphitizability of Carbon Materials Using Graphene and Graphene Oxide**

M. Singh, R. Vander Wal

Heat treatment of carbon is an age old process and has been extensively studied with an emphasis on identifying structural transformation dependence upon heat treatment temperature. This heat treatment can result in the formation of carbon of the graphitizable or the non-graphitizable variety. While a graphitizable carbon forms graphite on heat treatment at 2600 °C, a non-graphitizable carbon shows the presence of odd membered rings. The focus of this study is to determine the structure and cause of cross-links that result in non-graphitizability. The exact nature of cross-links responsible for non-graphitizability are still unknown. Monitoring the materials trajectory with respect to time at temperature can provide insight into the nature and formation mechanism of cross-links found in heat treated non-graphitizable carbons. Prior to graphitization heat treatment, carbonization of organic precursors is done at a relatively low temperature of 500°C to form carbonaceous material. Carbonization of solid and liquid precursors results in the formation of a coke or a char, with the primary difference being their formation pathway. A coke passes through a liquid-crystal state and forms a
carbon of the graphitizable kind while a char does not. The non-graphitizability of chars formed from oxygen rich precursors is believed to be due to the formation of odd membered rings, predominantly pentagonal, upon the evolution of oxygen atoms during carbonization. Subsequent graphitization heat treatment of these materials results in a fullerene-like nanostructure. To test this, graphene and graphene oxide are used as model materials with the latter being representative of a non-graphitizable carbon owing to the presence of oxygen groups. Both of these materials are mixed with anthracene, a graphitizable carbon, carbonized and further subjected to traditional furnace heat treatment at 2600 °C. Physical and chemical transformations of the resultant materials formed by annealing were measured with energy dispersive X-ray spectroscopy, selected area electron diffraction, and electron energy loss spectroscopy. Virgin samples and furnace annealed samples available in bulk were analyzed with X-ray diffraction. To resolve the detailed morphological and nanostructural changes, high resolution transmission electron microscopy is used to examine the carbons before and after annealing.

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Energy Savings with Microwaves: Metal Powder Heating Mechanisms


Microwave processing can produce superior properties of materials with significant time and energy savings, plus less pollution and waste, making it an environmentally friendly technology. Mechanisms by which metal powders heat rapidly in a microwave field are complex and not well understood, but our recent experiments with copper powder have shed new light on the mechanism. An improved power loss equation is presented.

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Advanced Multifunctional Coatings and Materials Processing for Extreme Environments


Research activities include the synthesis, processing, and characterization of nano, multilayered, nanostructured, functional graded, ceramic, and metallic coating systems with novel design architectures deposited by reactive and ion beam assisted deposition (IBAD), electron beam physical vapor deposition (EB-PVD), cold spray, thermal spray technologies, chemical vapor deposition (CVD), cathodic arc, sputtering (r.f, d.c., magnetron), plating (Ni, Cu, Pt), hybrid processes, and various other PVD processes. Present work includes the enhancement of coating microstructure and composition to tailor and improve the properties of vapor deposited coatings such as thermal barrier coatings, erosion resistant coatings, wear resistant, corrosion resistant, diamond like carbon, transition metal nitrides, carbides, and borides, and transition and rare-earth metal oxides for a variety of applications in the aerospace, tooling, nuclear, power, oil and gas, biomedical, and defense industries under extreme environments. Additionally, recent research interests include development of metamaterials, low friction coatings, antimicrobial coatings, smart coatings, failure analysis, and corrosion-resistant and wear-resistant material systems for oil and gas industry. Primary area of interest includes the development and processing of monolithic, nanocomposite, and multilayer vapor deposited coatings, nano-grained structural materials, and nano-layered coatings for extreme environments, as well as materials characterization using a variety of techniques.
analytical techniques. These material advancements contribute to a variety of applications in the aerospace, defense, tooling, power, biomedical, and optical industries. They represent the convergence of research driven by materials science and engineering with an applied nature.

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Development of Sacrificial Coating for Magnesium Aerospace Components

K. S. Venkataraman, R. W. Gresh, B. A. Shaw, E. Sikora

With the development of newer magnesium alloys for aerospace applications, a greater emphasis needs to be placed on designing sacrificial coatings for protection of these alloys. Non-equilibrium vapor deposits of magnesium exhibit a more ‘active’ nature as compared to the bulk alloys. With only ‘one phase’ constituting the entire coating, physical vapor deposits of certain magnesium alloys exploit the preferentially corroding nature of magnesium to produce better candidates for sacrificial coatings. Vapor deposits of pure magnesium and rare earth containing magnesium alloys (WE43, EV31) showed promising results on silicon substrates. Vapor deposits of WE43 had a corrosion rate of 8.2 mpy (in 0.1M NaCl and measured against SCE) and an open circuit potential of -1.88 V as compared to its bulk corrosion rate of 21.1 mpy and an open circuit potential of 1.66 V. As we transition from silicon to AZ61 substrate, post deposition heat treatment and specimen surface preparation affect the adhesion and hence the electrochemical behavior of the vapor deposits. Vapor deposits of WE43 on AZ61 substrate after post deposition annealing exhibited a corrosion rate as low as 1.5 mpy. While atomic emission spectroscopy gave us the elemental composition of the vapor deposits, scanning electron microscopy gave an insight to the morphology of the vapor deposit. Both techniques, in addition to electrochemical characterization, contact angle measurements and porosimetry combine to give a holistic insight to the corrosion mechanisms in the vapor deposits. Our vapor deposits have a more negative open circuit potential and a lower corrosion rate – however, as we transition to a real life application, we wish to preserve those characteristics if not better it. Ion beam assisted physical vapor deposition can improve the adhesion by increasing the number of nucleating centers while fluoridization can create a ‘self-healing’ top layer. We look to incorporate these techniques as we transition to real life applications.

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Application of Mesoporous Materials for CO₂ Capture and Conversion

X.X. Wang, X. Jiang, N. Koizumi, C.S. Song

Currently about 80% of energy worldwide comes from coal, oil, and natural gas, the combustion of which accounts for over 85% of total CO₂ emission. Carbon capture and utilization is of critical importance in mitigating the greenhouse gas effect while meeting the increasing global energy demand and achieving the target of the Paris Agreement. To confront the challenge, we have developed solid sorbents for CO₂ capture and metallic catalysts for CO₂ conversion with the utilization of mesoporous materials. A new concept called molecular basket sorbents (MBS) has been proposed for developing solid sorbents consisting of functional polymers immobilized in a nano-porous matrix such as SBA-15, which shows high selectivity (CO₂/N₂ > 1000) and high capacity (> 140 mg-CO₂/g-sorb) for CO₂ capture from various gas mixtures including flue gas of electric power plants. For CO₂ conversion, a series of Pd catalysts supported on mesoporous molecular sieves has been developed and evaluated for methanol synthesis from CO₂ hydrogenation. Compared to the conventional amorphous silica, the use of mesoporous support can confine the growth of small Pd nanoparticles, leading to higher activity for CH₃OH formation.
Tailoring Microstructure and Processes to Enhance Structural and Functional Properties of Ceramic Materials


The structural and functional properties of ceramic materials are determined by their microstructure. Key parameters are grain size and shape, crystallographic orientation of the grains, as well as grain boundaries characteristics. These factors are controlled by the material processing.

The Messing group investigates a variety of processes, from the rheological behavior of slurries during casting techniques to the sintering and high temperature processing, in order to develop a fundamental understanding of interface processes and mechanisms responsible for densification and microstructural evolution in ceramics. For instance, tailoring of microstructures through controlled Templated Grain Growth (TGG) has been a breakthrough in our research group, which has led to producing textured piezoelectric ceramics with functional properties close to single crystal materials. The TGG process is typically used in conjunction with shear forming techniques, such as tape casting, that align anisotropic template particles to control grain growth and crystallographic orientation.

Recent research based on advanced forming techniques, such as co-casting, are currently being explored to produce microstructural composites, i.e. bulk ceramics with different microstructures in different regions of the material, which feature superior mechanical properties for structural applications. By studying the relationship between slurry rheology, sintering, and microstructure development, we gain a deeper understanding of the science behind how processing drives structure-property relationships that yield unique properties (e.g. optical, mechanical or electrical) that we observe in ceramics.

New Polymeric Materials for Additive Manufacturing

M. A. Hickner Research Group

New materials are needed to realize the promise of additive manufacturing. The Hickner Research Group has applied their tools of polymer synthesis and detailed materials characterization to the formulation, fabrication, and analysis of new polymers processed using additive manufacturing techniques. This poster will detail our current work investigating both thermally processed materials as well as photopolymers that are used in stereolithography. We have highlighted a few projects on composites, polymer membranes, and responsive materials. Our future work is aimed at exploring materials and composites that cannot currently be processed using additive means and to expand the pallet of materials and properties available from additively manufactured components.

Functional Polyolefins with High Thermal Stability

G. Zhang, W. Zhu, M. Chung

The limitation of thermal stability in PE and PP polymers causes concerns in maintaining low operational temperature. Industrially, hindered phenol compounds are always used as antioxidants in polyolefin materials, including octadecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)-propionate (Inganox 1076) and pentaerythritol tetrakis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate] (Inganox 1010). Since these stabilizers are polar antioxidant molecules, it is difficult to achieve a homogeneous mixture. Moreover, these small molecule antioxidants are prone to run to the surface of polymer, resulting in the loss of antioxidant when exposed to solvents or heat.
We report a new class of functional polypropylene (PP-HP) and polyethylene PE-HP copolymer containing a PP backbone and various concentrations of hindered phenol (antioxidant) moieties which are located in the pendant side chains. An effective synthesis route has been developed to prepare these semicrystalline PP-HP and PE-HP copolymers with well-controlled microstructures, including tapered and random copolymers. Evidently, these PP-HP and PE-HP polymeric stabilizers show the cocrystallization phenomenon with the PP and PE homopolymer, which provides an ideal mechanism for introducing a high concentration of HP antioxidants that are homogeneously distributed and immobilized in the PP amorphous matrix.

PP-HP and PE-HP copolymers show significantly higher thermal-oxidative stability than the commercial PP and commercial PE products that contain a small amount of organic hindered phenol stabilizers. The combination provides PP-HP and PE-HP copolymers and their PP-HP/PP PE-HP/PE blends with exceptionally high thermal-oxidative stability that is tunable by the incorporated HP content. This new antioxidant mechanism is particularly beneficial in the long-term protection of PP and PE products under severe application conditions.

In addition to the known advantages of polymer-bonded stabilizers, with low mobility and volatility to prevent loss through diffusion and/or extraction (particularly acute in films and coatings), the PP-HP thin dielectric films with uniform morphology show a higher dielectric constant and maintain low dielectric loss, particularly for the tapered PP-HP copolymers with high crystallinity.

Non-linear dielectrics such as ferroelectric, antiferroelectric, and paraelectric materials play a crucial role in the functionality of integrated circuits, capacitors, and energy storage devices. Especially due to their intrinsic polarization mechanisms resulting in high permittivity and low loss, they are the most suitable material platform for extreme operation conditions in terms of temperature, voltage, and frequency. While pristine devices often exhibit desired and predictable properties, under field stress oxygen vacancy migration leads to resistance degradation and a spatial distribution of conductivity within the dielectric. Recent research efforts also identified the impact of the electrode/dielectric interface and defect complexes to effect the resistance degradation process of single crystals strongly. In addition, grain boundaries in polycrystalline materials are known to impede the resistance degradation process, but little is known about the impact of one specific grain boundary. The study of bicrystals is a suitable approach to gain information about the effect of a single, specific tilt or twist boundary on the local conductivity during degradation. Along with the experimental studies, a predictive hierarchical multi-scale simulation approach is developed that allows a fundamental understanding of what controls the above introduced degradation and breakdown mechanisms. The poster will present a summary of different experimental and computational approaches to investigate the role of the electrode/dielectric and grain boundary
interface carried out as a collaborative study with researches at Penn State, NC State University, University of Virginia, and TU Darmstadt. Specific key findings are highlighted that are anticipated to lead to improved predictability of device behavior and increase their reliability.

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**Steep Slope 2D Strain Field Effect Transistor: 2D SFET & Electro-ablated Monolayer TMDs**

D. S. Schulman, A. J. Arnold, S. Das

In this poster, we provide insight into the recently proposed two-dimensional (2D) electrostrictive field effect transistor or 2D-EFET, which employs strain induced dynamic bandgap engineering in 2D layered semiconductors to achieve sub thermionic and steep slope switching. In particular, we investigate a more realistic structural derivative of the original 2D-EFET and employ piezoelectric material as the gate insulator for strain transduction upon the application of gate voltage. We refer to this derivative as two-dimensional strain field effect transistor or 2DSFET. The out-of-plane compressive stress on the 2D semiconducting channel dynamically reduces its bandgap. This effect coupled with the field effect action achieves internal voltage amplification leading to sub-60mV subthreshold slope while maintaining ON/OFF current ratio of more than 10^6, and achieving ~2X higher ON current compared to the conventional 2D FET.

We also report a facile, high yield synthesis technique for obtaining monolayers of a wide variety of 2D materials, including MoS\(_2\), WS\(_2\) and MoSe\(_2\), from their corresponding bulk counterpart via an anomalous but elegant electrochemical corrosion process, also referred to as electro-ablation (EA). The electro-ablation (EA) process has key advantages over mechanical exfoliation and chemical vapor deposition (CVD) methods. Mechanical exfoliation results in extremely small, low yields of monolayers, whereas wafer scale CVD growth of high quality monolayers demand expensive equipment. We demonstrated high performance thin film transistors (TFTs) based on these EA monolayers with current ON-OFF ratios in excess of 10^7 along with ON currents of 120\(\mu\)A/µm for MoS\(_2\), 40\(\mu\)A/µm for WS\(_2\) and 40\(\mu\)A/µm for MoSe\(_2\), which outperform the existing TFT technologies.

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**Tunable and Flexible Metasurfaces**

X. Chen, X. Ni

The newly emerging metasurface is an ultra-thin layer of sub-wavelength elements (or a two-dimensional metamaterial) that locally tailors the electromagnetic field at the nanoscale, offering tremendous power for manipulating light. In addition, the abilities to bend or stretch the metasurface devices will open a new dimension to controlling electromagnetic waves. These abilities also promise a new way to design multi-functional devices which have different responses in different states. Here, we demonstrate a stretchable metasurface achieving intensity and phase modulation based on the resonance change of the underlying nanostructures. We use resonating nanoantennas on a flexible polydimethylsiloxane (PDMS) substrate to form a metasurface. By judiciously designing the nanoantennas, the resonance can be shifted when the substrate is bent or stretched. We are able to modulate the reflectivity from zero to unity using such a metasurface and to achieve phase tunability covering the whole 2\(\pi\) range of reflected electromagnetic waves. The demonstrated approach gives the way for achieving compact tunable perfect absorbers and dynamic beam steering.
Interfacial Chemistry
Regulation Via a Skin-Grafting Strategy Enables High-Performance Lithium-Metal Batteries

Y. Gao, Y. Zhao, Y. C. Li, Q. Huang, T. E. Mallouk, D. Wang

The lithium (Li) metal anode suffers severe interfacial instability from its high reactivity towards liquid electrolytes, especially carbonate-based electrolytes, resulting in poor electrochemical performance of batteries that use 4-V high-capacity cathodes. We report a new skin-grafting strategy that stabilizes the Li metal-liquid electrolyte interface by coating the Li metal surface with poly((N-2,2-dimethyl-1,3-dioxolane-4-methyl)-5-norbornene-exo-2,3-dicarboximide), a chemically and electrochemically active polymer layer. This layer, composed of cyclic ether groups with a stiff polycyclic main chain, serves as a grafted polymer skin on the Li metal anode not only to incorporate ether-based polymeric components into the solid-electrolyte interphase (SEI) but also to accommodate Li deposition/dissolution under the skin in a dendrite/moss-free manner. Consequently, a Li-metal battery employing a Li metal anode with the grafted skin paired with LiNi0.5Co0.2Mn0.3O2 cathode has a 90.0 % capacity retention after 400 charge/discharge cycles and a capacity of 1.2 mAh/cm² in a carbonate-based electrolyte. This proof-of-concept study provides a new direction for regulating the interfacial chemistry of Li metal anodes and for enabling high-performance Li-metal batteries.

Integrating 2D Materials and Nanostructures for Photonic and Medical Applications

S. Huang

Two-dimensional (2D) materials have gained tremendous attention in recent years due to their great potential for applications in large-area and flexible electronics, optoelectronics, and thermoelectrics. To realize high-performance devices, the fundamental study of material properties as well as the exploration of the integration of 2D materials and other nanostructures are necessary stepping-stones. Prof. Shengxi Huang’s research group at Penn State has multidisciplinary experience in experimental physical chemistry, optical spectroscopy, and photonics for 2D materials and nanostructures. We focus our research on nanoelectronics and nanophotonics for next-generation computing, sensing, and medical technology by exploring the following aspects, which are original and important in advancing the fields of nanomaterials and nanoscience.

1. **Fundamental study of 2D materials: anisotropic dynamics, near-field spectroscopy**

The optimization of 2D material-based devices is guided by the fundamental optical properties, including stability, dynamics, anisotropy, and exciton/trion behaviors. We aim at gaining a better understanding of these properties of 2D materials including graphene, transition metal dichalcogenides (TMDs), black phosphorus, iron-based superconductors. We will use various optical spectroscopic and microscopic tools, including Raman, photoluminescence, absorption spectroscopies, ultrafast optics, and scanning near-field optical microscopy, to examine surface defects, crystal boundaries, phase change, and electromagnetic field distribution in integrated materials.

2. **Integrating 2D materials and nanostructures: quantum confinement and tuning**

2D materials possess many unique properties not existent in their conventional 3D counterparts. The coupling of these properties with other nanostructures,
such as nanoparticles and metamaterials, can yield novel quantum phenomena. In particular, we are interested in (1) quantum confinement effect using 2D materials and metal nanoparticles, and (2) hybrid 2D materials with tunable hyperbolic polaritons. These works will facilitate the study of high-resolution far-field imaging and field enhancement, new quantum optics enabled by 2D materials such as photonic topological insulator, single photon emission, photon-entanglement, and super-radiance.

3. **Optoelectronic and medical applications of 2D materials and integrated structure**

In the application part, we are interested in two aspects. (1) 2D materials integrating metasurfaces and self-assembled 2D heterostructure for novel electronic and optoelectronic devices, including synaptic, tunneling, and infrared devices, which have the advantages of distinguished performance, high efficiency, ultra-flexibility, simple fabrication, and reduced cost compared to their 3D counterparts. (2) Medical applications with molecule detection. 2D materials will be used in our newly-discovered Raman enhancement technology, and a disruptive new technology will be realized which brings a highly reliable, convenient, and inexpensive biosensing tool. Combining effective machine learning approaches, revolutionary technologies will be realized such as point-of-care medicine and effective cancer prediction.

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**Dielectric and Viscoelastic Properties of Electrostatic Network Ion Gels**

J. E. Bostwick, C. Zanetolli, L. A. Madsen, R. H. Colby

Imagine a non-flammable solid with the modulus of plexiglass, but where a high density of ions are mobile as if they were in still in a liquid. Last year a new class of materials, termed electrostatic network ion gels (ENIGs), was discovered with a revolutionary combination of properties that could be utilized for electrochemical devices. These conducting solids, formed from a lyotropic nematic phase of a magnetically aligned rigid-rod polyanion, a sulfonated aramide, and an ionic liquid (IL) exhibited an unprecedented combination of ionic conductivity, widely tunable modulus, and thermal stability. In our study, we employed oscillatory shear rheology and dielectric relaxation spectroscopy to analyze ENIGs of varying polymer content, 4–13 wt.%, with 1-butyl-3-methylimidazolium tetrafluoroborate IL. By increasing the weight percent of polymer content in the ENIGs, the storage modulus increased from 0.2–4 MPa while reaching an ionic conductivity of up to 4 mS/cm at room temperature. ENIGs thus overcome the usual compromise between ionic conductivity and modulus in solid-polymer or composite electrolyte systems, demonstrating their potential to resolve current limitations in Li metal batteries, allow for safer operation, and generate 2–3X higher energy density than existing Li batteries.

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**Space-time Modulated Metasurface**

X. Guo, X. Ni

Nonreciprocal components such as optical isolators and circulators are essential building blocks for optical communications and computing. They allow the propagation of light in one direction while blocking that in the opposite direction, thereby reducing the undesirable reflections and preventing interference problems. However, most optical components are made from natural materials that have linear and time-independent properties, which are inherently constrained by Lorentz reciprocity. In order to break this limitation, we introduce
a space-time modulated metasurface which not only preserves the capability of spatial phase manipulation, but also offers a new degree of freedom resulted from temporal modulation upon light. We show theoretically and experimentally that the dynamic modulation produces a large space-time dependent phase change, and provides wavevector and frequency shifts upon incident light, hence creating a strong nonreciprocal effect. The phase modulation depth is greatly amplified by the resonant nature of the metasurface. Furthermore, unidirectional frequency shift is manipulated by the spatial phase gradient of the metasurface, which reduces unwanted sidebands and provides the flexibility of selecting conversion directions. Compared with bulky time-varying structures based on electro-optic and acousto-optic modulation, the space-time modulated metasurface exhibits a small footprint, a large modulation frequency of a few THz, and is compatible with current CMOS processes. We believe this nonreciprocal metasurface can work as optical isolator and potentially provides a viable new direction in constructing on-chip nonreciprocal optical components.

Recent Developments in the Fabrication of Astronomical Gratings

F. Grisé, J. McCoy, R. McEntaffer, D. Miles, N. Zhang

Developments in grating spectroscopy is one of the keys to opening a new discovery space in the field of astronomy, and particularly in X-ray/UV astronomy. We present recent advances made at Pennsylvania State University where we research and develop new ways to build large-format gratings (i.e. dispersive elements) by using techniques and tools that are traditionally geared towards smaller format products. This includes the techniques for preparation and fabrication of master gratings in single-crystal and amorphous silicon, such as lithography (laser-beam, electron-beam), reactive-ion etching, and wet etching. Successful replication of the master into many replicas is a challenge given the size of these gratings; our group has, however, been recently using substrate conformal imprint lithography with success.

Visible Switchable Optical Metasurface with Phase Change Materials

Y. Ding, Y. Duan, A.S. Gupta, R.E. Herbert, X. Ni

Despite the ability of emerging metasurfaces to manipulate light in ways beyond nature, the properties of metasurfaces always rely on predefined structures and are therefore static. Tunable metasurfaces have far-reaching potentials and significances in chip-based optical devices. One way to realize metasurfaces-based optical devices with rapid and local switchability is to involve phase change materials, in which their optical properties can be modulated by external factors like heat, electric field, and mechanical forces. Especially, vanadium dioxide (VO₂) behaves like a dielectric under room temperature and transforms into a metal at around 340K, which is a great material for building switchable optical devices. However, the reported devices work almost exclusively in the infrared region where the strong metal-dielectric transition happens. Here, we demonstrate by combining a plasmonic metasurface with VO₂ that we are able to achieve switchability in the visible range. The phase transition of VO₂ will shift greatly the resonance peak of the metasurface elements, and therefore changes dramatically its optical response. We show that both the reflectivity and transmittance of the hybrid metasurface can be modulated by over 100%. The study points out a feasible mean to utilize infrared phase change materials in the visible range and pave a way for future applications involving switchable optical devices.
Anti-reflection (AR) coatings are crucial for minimizing optical loss in high efficiency concentrating photovoltaic (CPV) systems; however, a high performance, environmentally-robust strategy for plastic optics such as acrylic Fresnel lenses remains an ongoing challenge for the CPV community. Here, we demonstrate simple, two-layer fluoropolymer AR coatings that reduce the solar spectrum-averaged (400<λ<1600 nm) reflectance of acrylic plastic from ~3.9% to ~0.4% over a wide range of incidence angles. The coating layers are fabricated via glancing angle deposition in a thermal evaporator and exhibit controllable nanoporosity due to self-shadowing that enables their refractive index to be continuously tuned from n=1.31 to n=1.15 depending on the deposition angle.

Owing to their fluoropolymer nature, the films exhibit very low dispersion and are transparent deep into the ultraviolet down to λ~200 nm.

The resulting AR coatings adhere strongly to common optical plastics such as polymethylmethacrylate and polycarbonate and survive repeated mechanical bend and compression cycles on substrates flexed to 1 cm radius. The coatings are also extremely hydrophobic, with a water contact angle >140° that supports anti-fogging and self-cleaning behavior, and they are unaffected by prolonged sonication in most organic solvents, acids, and bases. They exhibit no deterioration in AR performance after ten days of damp heat testing (T=85°C and RH=85%) nor after one month of continuous (ongoing) rooftop outdoor exposure in central Pennsylvania. The coatings have been successfully applied to a variety of curved lens surfaces, with virtually no variation in AR performance for f-numbers as low as f/1. In particular, coating both sides of an f/2 acrylic Fresnel lens increases its solar spectrum-averaged transmittance from approximately 92% to 98%. Taken together, these results represent a significant development for plastic optics commonly used in CPV systems as well as more generally for broadband AR applications that demand extreme environmental, chemical, and mechanical durability.

The Penn State Applied Research Laboratory’s Electronic Materials and Devices Department (EMDD) has developed a vertically integrated capability from material synthesis through device fabrication and testing for DoD and commercial applications related to piezoelectric transducers, RF and power electronic systems, Chem/Bio sensors, and IR detectors.

This poster describes the range of crystal growth techniques, material synthesis capabilities, material characterization methods, device design and fabrication capabilities, and device testing used to support internal research projects and industrial collaborations. Recently expanded capabilities for ceramics processing and two-dimensional materials will be highlighted.

A series of specific examples of prototype materials and devices currently under development including single crystal and textured ceramic piezoelectric transducers, FETs, IR and radiation detectors, SiC diodes, semiconductor diodes, and MEMs structures will be presented.
| 90 | High Thermal Stability OLEDs |
|--------------------------------|
| J. S. Price, B. Wang, Y. Shen, N. C. Giebink |
| Reliability remains an ongoing challenge for organic light emitting diodes (OLEDs) as they expand in the marketplace. The ability to withstand operation and storage at elevated temperature is particularly important in this context, not only because of the inverse dependence of OLED lifetime on temperature, but also because high thermal stability is fundamentally important for high power/brightness operation as well as applications such as automotive lighting, where interior car temperatures often exceed the ambient by 50°C or more. Here, we present a strategy to significantly increase the thermal stability of small molecule OLEDs by co-evaporating an amorphous fluoropolymer that stabilizes their morphology and prevents crystallization. Using this approach, we demonstrate that the thermal breakdown limit of common electron and hole transport materials can be increased by more than 50°C with minimal impact on their electrical transport properties. Simple bilayer OLEDs fabricated using this technique are shown to be functional at temperatures up to 250°C. The generality of our approach points toward a new class of thermally robust and morphologically-stable organic electronic devices that are capable of operating or being stored in extreme thermal environments. |

| 91 | Record-low Contact Resistances to Many Semiconductors |
|--------------------------------|
| K. A. Cooley, T. N. Walter, A. C. Domask, A. Molina, A. Agyapong, C. Lawrence, L. Kerstetter, S. E. Mohney |
| With decades of experience researching and developing electrical contacts to semiconductors, our group has achieved many record-low values of contact resistance and contributed to the scientific understanding of metal/semiconductor interfaces. In this poster presentation, we will review our work and highlight our latest findings on contacts to transition metal dichalcogenides and phase change materials. |

| 92 | Synthesis and Characterization of Advanced Nanoscale Materials |
|--------------------------------|
| S-Y. Yu, A. C. Domask, T. N. Walter, I. Campbell, K. A. Cooley, A. Molina, L. Kerstetter, R. Alsaadi, S. E. Mohney |
| Our group prepares and characterizes a wide variety of advanced nanoscale materials, especially metals and semiconductors. This poster presentation describes how we use (plasma assisted) atomic layer deposition and advanced microscopy techniques to prepare and characterize novel materials with characteristic lengths on the order of nanometers. |
Many applications from industrial electronics to medical devices benefit from close integration of electronics. In most cases today, the electronics is in the form of printed circuit boards populated with integrated circuits (ICs). But moving the electronic function from boards and ICs and more directly into the application can bring advantages. Thin film electronics, extensively developed for flat panel displays, provides a path to directly integrate transistors and electronic circuits with sensors, actuators, microelectromechanical devices, and more. We are developing zinc oxide (ZnO) thin film transistors (TFTs) and circuits for such applications.

Oxide semiconductor TFTs offer significant performance improvement compared to hydrogenated amorphous silicon (a-Si:H) devices, including $>10^6$ higher field effect mobility. ZnO semiconductor TFTs provide low-temperature processing, large field-effect mobility, and good electrical stability. Using low-temperature plasma enhanced atomic layer deposition (PEALD), Al$_2$O$_3$ gate dielectric and ZnO channel regions can be deposited at $<200 \, ^\circ \text{C}$. This allows ZnO TFTs to be fabricated on a variety of substrates, including glass and flexible polymeric materials.

PEALD ZnO TFTs fabricated on thin (\textasciitilde 5 \textmu m thick) polyimide substrates have characteristics very similar to devices fabricated on glass, with linear region field effect mobility $>10 \, \text{cm}^2/\text{V}[\text{Symbol}]\text{s}$ at a gate electric field of 2 MV/cm, and $i_{\text{on}}/i_{\text{off}} >10^8$. These devices survive tens of thousands of cycles of flexing or movement over few mm diameter rollers [1,2]. Al$_2$O$_3$ passivated devices have excellent device performance and stability, and double-gate and tri-layer TFTs provide additional design flexibility. Low-temperature processing also allows simple heterogeneous integration with piezoelectric materials such as Pb(Zr$_x$Ti$_{1-x}$)O$_3$ (PZT) and with two-dimensional transition metal dichalcogenide (2D-TMD) materials.

We are investigating ZnO TFTs in a range of applications. For example, we are integrating ZnO TFTs with PZT actuators to provide mirror figure correction for a future space-based x-ray telescope. The robust radiation exposure characteristics of ZnO TFTs simplify use in space applications. We are also investigating using ZnO TFTs as biosensors. For this application the ultrathin channels (typically <10 nm thick) used for our devices can provide sensitivity similar or better than nanowires or carbon nanotubes, but with greatly improved device reproducibility and stability. The flexible processing and design characteristics of oxide semiconductor devices provide advantages for these and many other applications.
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Direct Growth and Transport Properties of Epitaxial Graphene/Molybdenum Disulfide Lateral Heterostructures

D. D. Deng, S. Subramanian, K. Xu, N. Simonson, J. Li, D. Waters, K. Zhang, K. Wang, R. Feenstra, S. Fullerton-Shirey, J. A. Robinson

Low resistance contacts to the material is necessary to fully utilize the unique physical and electronic properties of transition metal dichalcogenides (TMDs) in devices. Graphene is a promising candidate and has been demonstrated to produce low-barrier contacts to MoS$_2$. Direct growth of graphene-TMD vertical heterostructures have demonstrated that such methods are advantageous for devices due to the cleanliness and scalability of the process. Recently, direct growth of graphene-TMD lateral heterojunctions has been demonstrated but limited to chemical vapor deposition grown graphene, which is intrinsically p-type and still requires physical transfer of the material. Here, we demonstrate completely transfer free, directly-grown epitaxial graphene (EG) - MoS$_2$ heterostructures. In addition, EG can be made n-type or p-type, and we observe that the type of the graphene heavily affects the heterostructure device performance. Devices with EG contacts of either type to the n-type MoS$_2$ exhibit steeper turn-on and larger on/off ratio compared to devices with metal contacts, but devices with n-type EG had significantly improved performance with an order of magnitude lower contact resistance, order of magnitude higher on/off ratio, and faster turn-on compared to metal contact devices. Exfoliated devices made using the EG shows approximately equal on/off ratio, but has a three-fold increase in the subthreshold swing, demonstrating the advantage of directly grown heterostructures. Barrier to electron transport for the directly grown devices extracted using low energy electron reflectivity shows that the device performance trends negatively with barrier height. This suggests the method can be extended to other TMDs by choosing the appropriate graphene type for low barrier junctions.

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Tuning the Dielectrophoretic Assembly of Dielectric Particles Through Surface Functionalization

N. Burrows, N. Alexander, I. Ibrahim, C. Keating

The directed self-assembly of particles in a non-uniform electric field can be achieved due to the phenomenon of dielectrophoresis resulting in an applied force. The strength of this force depends on the polarizability of both the particles & suspending medium, the particles’ size and shape, and the frequency of the electric field. The Clausius-Mossotti Factor, a frequency dependent function of both the particle and medium complex dielectric constant, determines the direction and magnitude of particle response to applied AC fields and changes with charge carrier density. Surface functionalization can alter the mobility of the charges associated with the particle surface electrical double-layer and presents an opportunity to further tune the dielectrophoretic (DEP) response. Herein, we present the DEP assembly of particles tuned by various surface chemistries and demonstrate the importance of surface charge mobility in DEP assembly.
Major challenges have emerged as microelectromechanical systems (MEMS) move to smaller size and increased integration density, while requiring fast response and large motions. Thin film piezoelectrics provide required large motions that can be generated, often with low hysteresis, the high available energy densities, as well as high sensitivity sensors with wide dynamic ranges, and low power requirements. The Trolier-McKinstry group has explored a wide range of perovskite thin films for these applications and has developed new characterization tools for measurement of thin film piezoelectric properties. Of particular interest is the development of high actuation authority films which are CMOS compatible both in terms of the required drive voltages and the processing temperatures. Patterning approaches, including reactive ion etching, and microcontact printing, are also being explored. A wide variety of piezoelectric MEMS devices have been fabricated, including:

1. Adaptive optics systems incorporating piezoelectric MEMS have been developed for a range of wavelengths, from the visible to the x-ray regime to produce local deformation of a mirror surface, in order to correct figure errors associated either with fabrication of the component or atmospheric distortion. High yield piezoMEMS arrays using PZT films were achieved on glass with a 220 nm radius of curvature. The resulting mirror pieces exhibit a consistent high yield of ~95%, with typical PZT dielectric loss values of 0.05 and permittivity of ~1270.

2. Micro-ultrasound transducer arrays have been developed to improve detection of disease and pathological classification. It has been demonstrated that PZT PMUT can operate in transmit and receive modes at high frequencies (30-70 MHz) with low drive voltages.

3. A high efficiency piezoelectric energy harvester operated at low resonance frequency and acceleration level was developed via bimorph textured PZT films on Ni foil. PZT films have stress tailored domain structures that provide efficient electromechanical conversion with high FoM.

In addition, we have developed new families of tunable dielectric materials, where the permittivity can be changed by the application of a dc bias field. The group was the first to demonstrate that Bi$_{1.5}$Zn$_x$Nb$_{1.5}$O$_6 + x$ (where $x = 0.5$ to 1) provide reasonable tunability (~50%) coupled with excellent temperature stability and low losses. Subsequently, it was shown that pulsed laser crystallization can be used to decrease the processing temperatures to 400°C, enabling integration onto polyimide.

Finally, in the area of bulk piezoelectric materials, the group worked to develop the cold sintering process to achieve high density at temperatures lower than conventional high-temperature sintering processing. A bimodal PZT powder was densified to a relative density of 89% by cold sintering at 300 °C and 500 MPa. After the cold sintering step, the permittivity was 200, and the dielectric loss was 2.0%. A second heat-treatment involving a 3 h anneal at 900 °C, increased the relative density to 99%; the resulting relative dielectric permittivity was 1300 at room temperature and 100 kHz. The samples showed well-defined ferroelectric hysteresis loops, having a remanent polarization of 28 µC/cm$^2$. 

V. A. A. Noel, R. A. Kimel

This project sought to investigate how the design of new material microstructures for clay might transform its properties to meet the need of sustainable housing in Ouagadougou, Burkina Faso. Clay (mud) is the typical material used in the construction of dwellings in Burkina Faso, because of its abundance, successful performance in the climate, and its familiarity within the culture. Our method involved carrying out on-site field observations of local brickmaking methods and building practices; visually and experientially examining two existing pilot houses; carrying out architectural analyses of their drawings and specifications; and doing material characterization tests of clay, concrete, and xyz brick samples used in building. We found that though insulation of the building envelope was addressed through the unit of brick (clay), other architectural issues such as roof design and construction, ventilation, and shading, to name a few, were not addressed to achieve thermal comfort in the pilot homes. Based on these results our next steps shall include: (1) Evaluating and analyzing the current building and design strategies of the pilot houses in Ouagadougou, Burkina Faso; (2) Developing architectural design strategies to address thermal comfort in the pilot homes; (3) Experimenting with engineered clay-based blocks for the creation of thermal performance figures of merit; and (4) Developing an “architectural design strategies guide” for sustainable dwellings in the region that takes the people, the context, and their resources into consideration.

Point-of-care Microfluidic Platform Using ZnO Nanowire Template for Virus Detection by Plasmonic Colorimetric Reaction


Here, we report a point of care (POC) microfluidic platform for virus detection by plasmonic colorimetric reaction. The size of PDMS-based device is about 2 cm × 2 cm × 0.5 cm, which is portable, cheap, and disposable. The integration of nanowires into microfluidic fabrication and the incorporation of nanoparticles for device operation ensure high virus capture efficiency, ultrafast and sensitive detection, and easy operation for multiplex virus detection. Plasmonic colorimetric reaction allows the estimate of virus concentration with naked eyes directly or by a cellphone-based imaging system for quantitative measurement. This POC platform enables fast detection of viruses outdoors in medical resource limited regions.

An antibody-virus-antibody ‘sandwich’ structure is utilized to detect virus. Antibodies conjugated on the surface of the device capture viruses, while antibodies conjugated with 13 nm gold nanoparticles target captured viruses for detection. Silver enhancer forms thick silver shells outside of the gold nanoparticles, allowing colorimetric reaction, which can be directly read with naked eyes or quantitatively analyzed by the greyscale of images. These grey values of the colorimetric reaction can reflect the concentration of virus. A cellphone imaging systems contains a camera surrounded with LED lights, and one pair of perpendicular polarizers, which helps eliminate specular reflection and enhance signal-to-noise ratio.

A novel process of replica molding of polymer polydimethylsiloxane (PDMS) directly from zinc oxide (ZnO) nanowire forests is invented to create an all PDMS device, which is highly biocompatible, has much large surface area and can significantly improve virus capturing efficiency and detection limit. Utilizing PDMS with uniform ZnO nanowires as the replica allows much larger rough surface
inside the channels, significantly improving virus capturing efficiency and pushing detection limit. The maximum height and roughness of the surface is larger than 1128nm and 163nm, respectively, with an increase of over 43% in surface area. The design of meandering channels and herring bone structures inside the channels increases the chance of interaction between antibodies on the surface and virus in the solution, which further raises the virus capture efficiency.

H5N2 avian influenza virus (AIV) solutions with concentrations from 2700 to $8 \times 10^5$ EID$_{50}$/ml are used to calibrate the standard curve of virus concentration versus grey values of the colorimetric reaction. The system pushes the detection limit of the virus to as low as ~8000 EID$_{50}$/ml, which is ~10 times more sensitive than the conventional enzyme-linked immunosorbent assay (ELISA) with fluorescence. What is more, the entire virus capture and detection process can be completed in 1.5 hours with a programmed syringe pump only. All of these make the device a user-friendly platform with higher sensitivity and easy detection.

### Expanding the Capacity to Confront the Global Water Crisis: Exploring Affordable Possibilities and Increased Effectiveness of Point of Use Ceramic Water Filters with Metallic Nanoparticles

I. Dabo, Z. Ounaies, S. Carpenter, II, S. Weitzner, F. Rodriguez

This study of ceramic water filters with metallic nanoparticles is an interdisciplinary collaborative effort, funded by the MRI Humanitarian Materials Initiative. The project seeks to advance a materials-enabled low-cost approach to provide clean water in remote areas. Our approach is comprised of a combination of computational, experimental, and testing capabilities to modify, adapt, or augment current point-of-use ceramic water filters to enable a wider range of filtration capabilities through the development of metal nanoparticle-modified ceramic materials. The point-of-use ceramic water filters are designed as a first response and temporary solution to provide clean water in remote areas where, although water is amply accessible, it is contaminated with waterborne disease and therefore unsuitable for consumption.

In this poster, we focus on the following research tasks: (1) experimental investigations of the effects of silver morphology, size and fabrication steps on the effectiveness of water filters to remove pathogens and metal impurities; and (2) first-principles modeling to understand the stability of active facets as a first step in predicting and evaluating the form of synthesized nanoparticles. This poster also reports on the following outreach and education tasks: (3) engaging one graduate student from Materials Science and Engineering, one graduate student from Art Education; two undergraduate students from Mechanical Engineering; two undergraduate students from Materials Science and Engineering; and one visiting international undergraduate student in Engineering; and (4) developing an interdisciplinary hypertext curriculum for K12 learners and an interactive web-based literature review and timeline of key concepts and developments in research and application of nanoparticle silver enhanced point of use ceramic water filters.
Smartphone-based Optical Spectrometer for Early Plant Disease Detection and Quantification


Developing low-cost, practical and accurate methods for early detection and quantification of plant diseases is a critical step toward achieving global food security. Here we demonstrate a solution for detecting plant diseases, in particular, the potato late blight disease by utilizing a smartphone based optical spectroscopic sensor. We measured diffuse reflectance spectrum data using a G-Fresnel smartphone spectrometer at Penn State Agricultural Experiment Station, and performed analysis based on machine learning algorithms including k mean and artificial neural network. Over 99% accuracy for quantifying the potato late blight disease was demonstrated in this preliminary study. Our results indicate that the mobile optical spectroscopic sensor platform provides a promising approach to early detection and quantification of plant disease non-invasively, at low cost, and with high throughput.

The Perceptions and Feasibility of 3D Printed Spectacle Design in Arusha, Tanzania

A. Cronin, M. Freeman, J. Rong, D. Zaremsky, E. Obonyo, S. Ritter, E. Park

The objective is to investigate the feasibility of increasing accessibility to prescription glasses in a resource-constrained context via the production and dissemination of 3D printed glasses. Eventually, we would like to produce durable and affordable 3D printed reading and prescription glasses. People in resource-constrained contexts are not receiving enough help with their vision issues. According to the World Health Organization, in 2014, 285 million people are estimated to be visually impaired worldwide, with 90% of them living in low-income settings. Forty-three percent of vision impairment is caused by uncorrected refractive errors, which can be corrected with prescription lenses. We believe 3D printing will increase accessibility to glasses by allowing both optometrist and consumer to operate in the eyewear market more efficiently through mass customization. For our objective, we sought to prototype 3D printed lenses and find out if the context has the resources and people to support the glasses. We have been able to print translucent lenses, but we still need to process them in order to make them clear.

We conducted 30 interviews in person in the Arusha area in Tanzania to learn about perceptions on eyewear and 3D printing. We interviewed workers and optometrists in three optical shops to learn about the price of receiving glasses along with the frame options. From the people interviewed, 73% stated that a barrier to accessible glasses is the cost. Out of those people, 30% say that awareness of vision problems and locational access are also barriers. Seventy-seven percent state that the cost of glasses is too high. Misconceptions about vision can be another barrier. Only half of the people interviewed stated that children who have vision problems should be given glasses. Some who disagreed believed that wearing glasses could bring harm to the children’s eyesight. Less than half were aware of what 3D printing is, though 80% were willing to purchase 3D printed glasses depending on factors such as the cost, availability, and quality. New prescription glasses were purchased for prices between $30 and $60.

In order for 3D printed glasses to be a feasible product, we recommend that the glasses not be more expensive than the cost of glasses currently in the market and that the 3D printed glasses have good quality and durability. Additionally, we would need to find a way to bring the glasses to rural areas and correct the misconceptions about vision impairment.
In the last couple of weeks, I have been blessed to be part of something bigger than myself. My colleague and I are considering the usefulness, or rather the lack of usefulness, of the peanut shell in the developing world. We choose to zone in on an area near Lake Victoria simply because it had fertile and favorable soil for the peanut plant to dwell in. Given this fact, we realized that 92% of peanut shell obtained from the peanut were discarded as trash. Within this we saw an opportunity to investigate the feasibility of creating a desirable ceiling board material locally. Keeping in mind that these weren’t very high-income people, our objective was to create low cost and low tech production locally, by turning the shell of a peanut from shell to powder, then to ceiling board. Our intention is to build a value chain out of a material that is currently being regarded as waste, then eventually moving into the formal construction sector. In doing so, we will help alleviate some of the impoverished peasant farmers by giving them more out of the peanuts they produce already.

We present an overview of IRG2, one of four Interdisciplinary Research Groups which comprise the Center for Nanoscale Science, Penn State’s MRSEC. IRG2 synthesizes and studies active matter at the nano-scale. These nanomotors consume energy to move through their environment – in this respect they resemble biological systems. The objects studied by IRG2 are much simpler than living systems; nonetheless, these synthetic motors exhibit many behaviors previously unique to living matter.

Systems studied represent a range of design (single enzymes, bi-metallic rods, light sensitive microparticles, functionalized polymer spheres ...) and motive mechanisms (self-electrophoresis, acoustic propulsion, light-activated catalysis, thermal gradients ...). Many of these self-propelling systems have dual applications as micro-pumps, generating flows in their environments when immobilized.

We present an overview of the IRG’s works from the past year. Among these are oscillatory and swarming behavior in silver phosphate colloids, preferential upstream movement (rheotaxis), small-molecule chemotaxis, and biocompatible propulsion mechanisms.

The Malvern Morphologi G3SE, recently acquired by MCL, is a high resolution microscope-based automated imaging system that can characterize particles ranging from 0.5 microns to several millimeters in size. Individual particle images are captured from dispersed sample and scanned across sample area underneath the microscope optics while keeping the particles in focus. As a result, particle size distribution and particle morphology are determined. One of the main advantages of automated imaging is that it provides statistically representative distributions by measuring 10’s to 100’s of thousands of particles per measurement. This technique can be used in conjunction with laser diffraction to gain a deeper understanding of the sample or to validate the laser diffraction method.

Proper sample dispersion is crucial for Morphologi measurements. This can be achieved by several dispersion accessories available in our lab including: (1)
software controlled dry powder sample dispersion unit (SDU) when sample is dispersed by an instantaneous pulse of compressed air with controlled dispersion pressure and injection and settling time; (2) 4-slide plate where samples can be dispersed by evaporative dispersion often used for highly cohesive particles; (3) glass wet cell that is designed to measure >15 micron particles in suspension, and (4) 25 mm filter plate suitable to study filtered material.

The purpose of this poster is to show the capabilities of Morphologi and how they have been used to solve research problems. The instrument is located in N-001 Millennium Science Complex.

CRAFT is the first multidisciplinary center devoted to advanced fiber technologies at Penn State. The center proposes to establish the foundation of next generation programmable, flexible, biocompatible, optically superior, energy efficient, and mechanically strong fibers. The research center is committed to educating internationally competitive scientists in fiber science and technology through cutting edge, interdisciplinary research programs. Penn State faculty from the College of Engineering, Eberly College of Science, College of Earth and Mineral Sciences, and the College of Agricultural Science are involved in the CRAFT center, which is coordinated by the MRI. The Center serves as the hub to attract diverse Penn State faculty and obtain substantial state, federal, and industrial funding in the new field of multi-functional advanced fiber technologies. The mission of CRAFT is to become an international leader in research on new phenomena and applications of programmable smart composite fibers that could be transformed into high impact functional textile products in medicine, automobile, energy, biotechnology, and cosmetic industries. The Center also provides a unique, vertically integrated research education to graduate and undergraduate students, with extremely valuable components, including state-of-the-art infrastructure and research environment.

The Two-Dimensional Crystal Consortium - Materials Innovation Platform (2DCC-MIP) is an NSF-funded national user facility (cooperative agreement DMR-1539916) focused on the development of two dimensional (2D) chalcogenides for applications in next generation electronics. These materials include 2D transition metal dichalcogenide films that are only a few atoms thick, topological insulator bismuth chalcogenide films that only conduct on the 2D surface, and multilayers of dissimilar chalcogenide films. There are three main components of a MIP: In-house Research, User Facility, and a focused Education and Outreach program related to the research.

The 2DCC user program focuses on three main facility components:

1. **Synthesis and In situ Characterization of Thin Films**
   This facility is focused on developing advanced synthesis tools for chemical vapor deposition and hybrid molecular beam epitaxy equipped with real-time, in situ characterization tools that probe the growth, electronic structure, and materials properties of atomically thin films.
2. **Bulk Crystal Growth**
This facility is focused on the bulk growth of layered chalcogenides to provide high quality crystals grown under near-equilibrium conditions.

3. **Theory/Simulation**
This facility is focused on supporting the experimental work with theoretical techniques including molecular dynamics simulations and reactive force-field modeling to address the complex kinetic issues surrounding materials synthesis.

Researchers from academia, government, and industry interested in participating in the 2DCC User Program can access the specialized samples, synthesis equipment, and simulation tools through several modes of interaction. Users can request a limited number of well-characterized samples free of charge through a brief on-line application which describes their needs and research interests. A list of available samples is posted on the 2DCC website. Users interested in accessing the capabilities of the 2DCC for more extensive research projects can do so via the submission of a brief research proposal which is evaluated by researchers external to Penn State.

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**Investigation of Surface Conditions on the Cooling of Nuclear Fuel Rods**  
**PSU Global Nuclear Power Safety (GNPS) Center**  
S. Ebrahim, F-B. Cheung

This research investigates the influence of surface conditions on the cooling process of nuclear fuel rods. Specifically, material characterization of CRUD formed on the fuel rod surfaces is performed and its effects on the cooling of fuel rods are studied. The term CRUD (Chalk River Unidentified Deposits) is used to describe the deposited corrosion products on the surface of the fuel cladding rods during the operation of Pressurized Water Reactor (PWR). The Pennsylvania State University has constructed and operated a 7x7 rod bundle test facility under the Rod Bundle Heat Transfer (RBHT) Program sponsored by United States Nuclear Regulatory Commission (NRC). Inconel type 600 rods with the dimensions of 9.5 mm diameter and 3.657 m heated length are used in the test facility. They have experienced an approximate of 200 total heating and cooling cycles under system pressure and cladding temperature ranges between 0.138 – 0.414 MPa and 315 – 1093 °C, respectively.

Material characterization has been performed on test samples collected at different elevations of the heated rods to identify the microstructures of the CRUD layers by using field emission scanning electron microscopy (FE-SEM), scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDS), and x-ray diffraction (XRD). Additionally, an automated goniometer and optical profilometry are used to measure, respectively, the surface roughness and the water contact angle of selected rod surfaces with and without CRUD formation. The goal is to correlate the surface conditions of the rods such as the surface roughness, the water contact angle, and the thickness, porosity and chemical composition of the CRUD layer on the cooling behavior of the rods under PWR accident conditions. A heat transfer correlation has been developed from the data which predicts the enhancement of the cooling process of the fuel rods following a severe accident such as loss-of-coolant-accident (LOCA) resulted in improving the safety of the PWR.
The Penn State Nanofabrication Laboratory (Nanofab) is a fully staffed user research facility offering more than 70 nanofabrication and characterization tools that enable fabrication and characterization of a wide range of devices to support fundamental and applied research. Researchers from Penn State, other universities, government labs, and industry take advantage of the expertise and world-class facilities of the Materials Research Institute’s Nanofabrication Laboratory.

Located in the Millennium Science Complex, the Nanofab provides faculty, students, and industry researchers access to sophisticated instruments for micro- and nanofabrication. The Nanofab’s 10,000-square-foot state-of-the-art cleanroom is supported by 6,000 square feet of space for utilities in the subfab. The Penn State Nanofab offers expertise in “top-down” (e.g. deposition, etching) and “bottom up” (e.g. self-assembling films) nanofabrication. The technical staff provides extensive support and training or can perform research on behalf of industry partners. More than 70+ materials can be deposited and dry etched in the suite of tools in the facility. The Lithography tools are capable of writing sub nanometer features on a variety of substrates, including curved surfaces. The laboratory is open 24 hours a day, 7 days a week, 365 days a year for trained users.

This poster highlights the state-of-the-art equipment that resides in the 10,000-square-foot cleanroom and the unique capabilities of the equipment. Recent additions to the lab include the highest resolution commercially available 3D printer; Nanoscribe Photonic Professional GT and the soon-to-be-installed latest generation SUSS MicroTec MA/BA6 Gen4 semi-automated mask aligner.

IRG4 seeks to understand and control the organization of particles and their mixtures to generate architectures in which non-additive functions are imparted by the collective properties of the array. Our multidisciplinary team of investigators includes experimental and theoretical expertise and spans engineering (Electrical, Chemical, Materials) and science (Chemistry, Physics, Materials). Several classes of assemblies are under investigation; these incorporate distinct types of functional particles and span a range of organizational ordering schemes for photonic applications ranging from metamaterials, whose function depends on controlled placement of metallic and dielectric components, to random lasers, which take advantage of disorder. Fabrication by solution-phase directed assembly of particles rather than top-down methods enables reorganization to switch between different functional forms. Learning how to achieve desired assembly outcomes for functional particles and their mixtures, and to reconfigure these assemblies in real-time, will set the stage for a new era of nanomaterial-enabled device applications.
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Center for Innovative Sintered Products – Fundamental and Applied Research in Sintered Materials
T. A. Palmer

The Center for Innovative Sintered Products (CISP) is an academic center focused on the development of cutting-edge technology for the processing of sintered material, particulates, refractory, and hard materials. CISP has focused on using research as an educational tool to involve students in contemporary problems associated with sintered materials. CISP research includes long– and short–term precompetitive and proprietary projects. Areas of emphasis include powder and particulate material characterization, sintering process development, tailored and functionally designed hard materials, thermal processing and measurement, and spark plasma sintering services.

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ATOMIC
M. Terrones, J. Robinson, N. Simonson, F. Zhang, K. Zhang, Y Lei

ATOMIC (the Center for Atomically Thin Multifunctional Coatings) is an IUCRC (Industry/University Collaborative Research Center) is led by Penn State in collaboration with Rice University. It is a collaboration between the National Science Foundation, a host of member companies, and Penn State and Rice to develop and apply two-dimensional materials (such as graphene, hexagonal boron nitride, and transition metal dichalcogenides) as coatings in a wide variety of fields.

The six main thrusts of ATOMIC are: Scalable Routes for ATOMIC, Protective Coatings, Energy Conversion & Storage, Reliability & Multifunctionality, Toxicology & Biocompatibility, and Water – Purification, Desalination, & Monitoring. Currently, most of these thrusts have at least one project exploring the potential of 2D materials for these technological challenges.

The IUCRC integrates academia, industry, and government/national labs to ensure the highest quality of relevant research led by professors such as Joshua Robinson (PSU), Mauricio Terrones (PSU), Jun Lou (Rice), and Pulickel Ajayan (Rice) as well as industry leaders such as Corning, Honda, Morgan Advanced Materials, and the Air Force Research Laboratory.

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3D Metal Printing in Penn State’s Center for Innovative Materials Processing Through Direct Digital Deposition (CIMP-3D)
T. Simpson

Penn State’s Center for Innovative Materials Processing through Direct Digital Deposition (CIMP-3D) serves as the Additive Manufacturing Demonstration Facility for DARPA’s Open Manufacturing. The facility offers state-of-the-art metal 3D printing capabilities in powder bed fusion and directed energy deposition along with hybrid manufacturing technology and computed tomography (CT) scanning. CIMP-3D’s mission is three-fold: (1) advance enabling technologies required to successfully implement AM technology for engineered components and structures; (2) provide technical assistance to industry through selection, demonstration, and validation of AM technology as an “honest broker”; and (3) promote the potential of AM technology through training, education, and outreach. With more than 45 faculty affiliates spanning five colleges, CIMP-3D uniquely positions Penn State as a “one-stop shop” for all aspects of additive manufacturing, including design, materials, modeling, simulation, sensing, post-processing, characterization, testing, inspection, and data management for qualification and certification. CIMP-3D offers tours to more than 1000 visitors each year and provides Penn State’s interface to America Makes, the National Additive Manufacturing Innovation Institute (NAMII).
Center for Dielectrics and Piezoelectrics (CDP)

S. Trolier-McKinstry, C. A. Randall

The CDP aims to provide international leadership and train next-generation scientists in the fundamental science and engineering that underpin dielectric and piezoelectric materials. The center supports industries based on capacitor and piezoelectric materials and devices through the development of new materials, processing strategies, electrical testing, and nanoscale characterization and modeling methodologies.

Innovations in the dielectrics and piezoelectrics industrial sectors often arise from research advances in materials chemistry, synthesis, and/or manufacturing that enable new materials and device functionality. A broad and diverse number of material challenges across the capacitor- and piezoelectric-based industries are addressed by research thrusts within the CDP. In many of these areas, the CDP faculty members are international leaders and have unique capabilities to drive research innovations for next-generation materials and devices. Our aim is to engage companies across the supply chain, i.e. ones that manufacture dielectric and piezoelectric materials, component manufacturers, and end users, who will provide the technological pull for CDP research activities.

CDP is a joint collaboration between North Carolina State University (NCSU) and The Pennsylvania State University (PSU) and is supported by the National Science Foundation and CDP members.

The Materials Computation Center - A Highly Versatile Faculty Collaborative for Computational Support of Materials Research


The Material Computation Center (MCC) represents around 20 faculty at Penn State involved in materials simulations, spanning many length scales – from highly accurate, small (<500 atoms) ab initio simulations all the way to CFD-simulations that directly affect macroscopic length- and time scales. At every size- and length scale MCC provides world-class capability – thus providing a highly versatile connection with the experimental capabilities in the other MRI centers. This poster highlights MRI-relevant research and features one of the unique methods within MCC - the ReaxFF method, which provides a highly transferable simulation method for atomistic scale simulations on chemical reactions at the nanosecond and nanometer scale. It combines concepts of bond-order-based potentials with a polarizable charge distribution.

The ReaxFF concept is transferable to applications to elements all across the periodic table, including all first row elements, metals, ceramics and ionic materials.

For all these elements and associated materials, we have demonstrated that ReaxFF can accurately reproduce quantum mechanics-based structures, reaction energies, and reaction barriers, enabling the method to predict reaction kinetics in complicated, multi-material environments at a relatively modest computational expense.

Recently, we have been developing and improving ReaxFF descriptions for various materials relevant to the Materials Computation Center and projects within the
Materials Research Institute (MRI). These include a capability to describe ferroelectric materials, simulation tools for CVD and ALD synthesis of chalcogenides and semiconductors, and supercritical water mixtures- with applications to cold sintering of zinc oxides and more complex oxide materials. In this poster we will highlight these new applications and their connections to ongoing MRI projects.

The 21st Century is facing several grand challenges in healthcare (such as antibiotic resistance issue, integrated diagnostics, etc.), sustainable energy, clean water, and food supply. In order to address these challenges, we need to make progress in multiple directions by understanding, predicting, and utilizing the involved parameters. Achieving so is only possible by a collaborative effort between communities in different areas of science and engineering.

At e-Bio-e lab, we work at the intersection of fundamental sciences (from material properties to cellular biophysics involved in diseases) with engineering of novel miniaturized systems to create point-of-care biochemical diagnostics and screening methods that are accessible to everyone, especially the low- to mid-income populations.

Toward these goals, we are interested in:

(i) Developing low-cost, array-formatted electrochemical devices on glass or plastics for detection of physiological and environmental factors in complex media (such as blood, urine, drinking water, etc.). We are particularly interested in healthcare application, including pathogen detection, antibiotic susceptibility testing, water quality screening, etc. (ii) Exploring different biomarkers (such as metabolites, reactive oxygen species, etc.) and novel materials (such as 2D materials, nanoparticles, porous materials, etc.) for enhancing the sensitivity. In this regard, we investigate the biocompatibility or toxicity of engineered nanomaterials, such as doped TMDs. (iii) On-chip devices for real-time study of cellular response to external input (such as light, chemical compounds, osmotic/electric/heat stress, etc.) and applying the findings as a basis to study diseases. (iv) Probing cell-cell communication with high temporal and spatial resolution. Some applications include monitoring the dynamics of lateral transfer of antibacterial resistance genes, host-pathogen interaction via organ-on-chip devices, etc.

We look forward to collaboration with other academic and industrial partners who are involved with: materials engineering (nanomaterials, organic materials, substrate materials, etc.), biological and medical sciences (cancer research, microbiology, tissue engineering, etc.), spectroscopy methods (fluorescence, Raman, etc.), surface chemistry (functionalization, biorecognition elements, etc.), system integration (microfluidics, IC design, wireless communication, etc.), and device modeling.
### 116
**Glass Research @ PSU**

**J. C. Mauro**

Glass Research at Penn State University covers a wide range of fundamental and applied glass science and technology. Topics include:

- Multiscale Modeling of Glass
- Viscosity and Fragility
- Glass Transition and Relaxation
- Glass Structure-Property Relationships
- Thermodynamics and Statistical Mechanics of Nonequilibrium Systems
- Decoding the Glass Genome
- High-Strength Glasses
- Glass Melting and Characterization
- Bioactive Glasses
- Exploratory Glass Compositions

This poster gives an overview of these research activities in fundamental glass science and advanced glass engineering.

### 117
**Additive Manufacturing of Metallic Materials**

**T.A. Palmer, Z. Khayat, S. Meredith, A. Iams, M. Brennan**

Additive Manufacturing (AM) is an iterative process that involves the fabrication of incremental layers directly from a Computer Aided Design (CAD) model. While AM has the potential to revolutionize material production through the development of innovative materials and the creation of parts with complex internal structures that are not practical using conventional methods, advancement of the technology will rely upon continuous efforts to improve the reliability and reproducibility of AM components. The goal of the Palmer Research Group is to establish greater process control through the development of a fundamental understanding of the governing process-structure-property relationships in additively manufactured metallic systems.

### 118
**Polyampholytes in Electric Fields**

**C. W. Pester**

Many diseases of the human nervous system occur as a result of neurodegenerative processes. Charged proteins – naturally occurring polyelectrolytes and polyampholytes – have been identified as key factors in the progression of diseases like Parkinson’s and Alzheimer’s. Research interests presented on this poster are focused on synthetically mimicking and studying the complex electrostatic interactions of such polyelectrolyte and polyampholyte architectures. Both provide a powerful platform for fundamental studies and simultaneously open new routes towards advanced materials that can be regulated via external stimuli, in both two and three dimensions, and for a variety of applications.

### 119
**Raman and Near-field Characterization of Graphene Heterostructures**

**M. Blades, X. Li, S. V. Rotkin**

Micro-Raman and scattering-type Scanning Near-field Optical Microscopy (s-SNOM) are well established nanocharacterization methods that can go beyond imaging mode: thorough analysis of the signals obtained can provide direct mapping of materials properties of 2D layered materials (graphene in this particular work). Single- and multi-layer graphene materials have been studied by Raman methods quite intensively, and good understanding of physics behind micro-Raman hyperspectral imaging was achieved. Current research expanded beyond bulk materials by studying heterostructures combining “infinite” 2D-layers with confined 1D- or 0D-objects (wires or dots). Here we present a few examples of such structures that hybridize the high quality CVD graphene,
transferred to other substrates, – a series of islands of a second layer, making natural bilayer heterostructures, or titania microcrystallites, or photonic metasurfaces. Both properties determined by graphene itself and by the other material in heterostructures influence the optical response, potentially resulting in plasmonic quantization, rotational incommensurability, strain induced effects – all attractive for future applications.

The Maria research group focuses on electronic materials belonging to the ceramic and semiconductor families. Historically, group research focused on non-linear dielectrics and insulators, but has broadened to cover nitrides, transparent conducting oxides, metallization, and carbides. Current “hot topics” in the Maria group include semiconductors for IR optoelectronics, entropy-stabilized oxides and carbides, reactive nanomaterials, oxide-nitride interfaces, and ultra-low temperature sintering. Maria group research is strongly application-inspired with an overarching focus on synthesis science. Active research areas in synthesis science include explorations of high power impulse magnetron sputtering, creating perfectly flat surface, near room temperature sintering, and entropic stabilization.

The application space of interest to the Maria group includes mid-wave infrared optical devices, including imagers, sensors, and overall improved “situational awareness”; tunable optoelectronic devices that merge ferroelectricity with transparent conductors; nanoenergetic materials that become components of advanced and safer military weapons systems; new approaches to pulsed power sputtering that enable improved film growth and coating; new platforms for tunable high mobility interface conduction; extreme high temperature materials development; and new materials for energy technologies based on entropic stabilization.

This poster will provide a summary of the Maria group research activities, the technologies of interest, our collaborations, and our laboratory infrastructure that will be developed at Penn State.

Non-Hermiticity in optics is associated with the presence of loss and/or gain. Engineering the interplay between gain, loss, and coupling strength among optical structures allows engineering their non-Hermiticity, and creates a variety of novel opportunities in photonics to generate, manipulate, and transmit light, and to control its interaction with matter. Using whispering-gallery-mode (WGM) microresonators as a platform, we have been investigating non-Hermiticity, including parity-time (PT) symmetry, in optics both for understanding the basic physics of non-Hermitian systems and the emerging degeneracies known as exceptional points (EPs) and for developing novel optical devices. Using the concepts of PT-symmetry and EPs, we have demonstrated (i) nonlinearity-based nonreciprocal light transmission in broken-PT regime with record low level optical power (ii) loss-induced suppression and revival of lasing, (iii) on-demand bidirectional and unidirectional emission in WGM resonators at EPs, and (iv)
enhanced optical sensing at EP beyond what is achievable in conventional resonator-based sensors.

This poster will present a brief overview of the Ozdemir Research Group’s efforts in the field of non-Hermiticity in optics and discuss future studies and potential applications. The poster will also present other photonic technologies that are being researched in the group, including the fields such as optomechanics (enhancement of amplification and cooling rates of mechanical motion), phonon amplification and cooling at EPs, quantum plasmonics, and single nanoparticle/molecule detection.

With plastic pollution on the rise, it is critical that we find sustainable alternatives in order to protect our natural resources. Replacing petroleum-based materials with low cost, biodegradable materials could have a tremendous impact on our environment and help the 21st century family go green.

Recent research at Penn State has demonstrated the ability of a PPC of carboxymethyl cellulose and chitosan to be used as an effective barrier coating material. However, little is known about the adhesive properties of this biocomposite. This work assesses the mechanical properties of bonded paperboard interfaces under both dry and submerged conditions. Initial results from single-lap shear tests under tensile force indicates considerable potential for this CMC-CS PPC as a natural adhesive.

In the manufacture of petroleum-based fuels and products, in the refining of ores, in the production of pharmaceuticals, polymers, and other materials, the multiphase flow plays an important role. During the manufacturing process, multiphase flow is the simultaneous flow of materials with different phases, which is commonly found to be turbulent flow. Understanding the fluid dynamic of turbulent flow and knowing the optimum conditions to set for producing desired flow can improve production efficiency and quality control of the industry. Lagrangian particle tracking (LPT) is a flow visualization technique for flow analysis and is frequently being used to forerun sophisticated quantitative measurements. The process of flow visualization often is the first step of obtaining a detailed flow analysis. It is crucial to have precise calibration to get an accurate measurement. Volume self-calibration and non-uniform optical transfer functions (OTF) are implemented in calibration to account for the adverse effects of optical distortions on tomographic reconstruction. The reconstruction calibrated to imaging conditions shows significant improvement regarding ghost particle intensity reduction and peak position accuracy to correct the mapping functions for all the cameras. These calibration techniques are integrated with iterative particle reconstruction (IPR), Shake-the-Box methods to enhance current Lagrangian particle tracking. This approach provides higher accuracy by virtually capturing more real particles and efficiently suppressing ghost particles formation. More reliable results up to 0.05 ppc can be generated with a greater...
level of target particles. LPT technique can also solve a broad variety of problems encompassing biomedical engineering, insect locomotion, and natural behaviors, energy dissipation analysis, uncertainty quantification, material behaviors, and global climate simulations such as ocean mixing.

A chiral sculptured thin film (Chiral STF) consists of an array of helicoidal columns with fixed pitch. Such films were fabricated out of zinc selenide using resistive-heating physical vapor deposition. During the deposition, the substrate was tilted at an angle of 20° with respect to the incident vapor flux and rotated as per the asymmetric serial bideposition (ASBD) technique. The pitch of each successive chiral STF was made to be double that of the previous chiral STF resulting in a total of five samples which act as polarization filters between around 732 nm and 11,712 nm. These samples were shown to reflect right circularly polarized light and transmit left circularly polarized light around a certain wavelength.

Post-harvest losses are a major threat to food and financial security for many countries in sub-Saharan Africa. In Tanzania, 20% of grain crops and 50% of fruits and vegetables spoil before they can be sold in the market. According to the 2007-08 Tanzania National Sample Census of Agriculture, Tanzania saw a total production of 18,866 tons of tomatoes, contributing the most (26%) to the fruit and vegetable sector of the market. However, between 20-50% of tomatoes harvested are wasted due to inadequate storage and transportation techniques. Refrigeration is the ideal solution to elongate the shelf-life of produce, specifically tomatoes. However, only 7% of the rural population is electrified with a variable electric source, leaving most farmers to turn to alternative, less effective storage methods. We have addressed this problem with the construction of a cold room designed with appropriate materials, utilizing both active and passive cooling techniques.

The Penn State Center for Nanotechnology Education and Utilization (CNEU) has established the Remotely Accessible Instruments for Nanotechnology (RAIN) Network. This growing group currently consists of 10 Universities, seven community colleges, and one secondary school district which are now providing effectual outreach and education activities via distance technology. A RAIN session allows students the ability to access and control characterization equipment, like field emission scanning electron microscopes (FESEM), and analytical tools, such as energy dispersive spectroscopy (EDS), to look at nanosized materials from the ease of classrooms all across the country. Students control the tools over the internet in real-time and with the assistance of an experienced expert advising over video conferencing software.

Power electronics aim at efficient energy conversion and regulation. Power semiconductor devices, PSDs, are at the heart of power electronics, enabling advanced distributed switch-mode power-supplies and increasingly replacing traditional devices. Like most solid-state devices, PSDs are used for rectification, amplification, and switching, with the major difference being handling high currents, high voltages, and typically operating in high-temperature environment. PSD applications range from hand-held devices to traction to high-voltage DC transmission. A special class of PSD is the MOS-controlled device. These devices
are advantageous in terms of their simple voltage control, high input impedance, and thermal stabilities. The silicon MOS-controlled power devices are the metal oxide semiconductor field effect transistor, MOSFETs, insulated gate bipolar junction transistor, IGBT, and Thyristor, dominating the low voltage, intermediate voltage and high voltage ranges respectively. The latest in device evolution of low voltage MOS-PSDs is the vertical U-shaped trench-gated MOSFET, UMOSFET, introduced in 1998 by Fairchild Semi Inc. and intensively researched at Penn State. As a switch, it handles high current in the ON-state, and high blocking voltage in the OFF-state. On one hand, the ON-state vertical current is tailored by the number of sources at top and flows to a common drain at the bottom. On the other, the blocking voltage is achieved through avalanche breakdown at the p-n junction region known as the drift region. The width of drift region is varied to tailor the blocking voltage value. On the fabrication side, the trench-gated region is formed by reactive ion etching of crystalline silicon wafer that result in bombardment damage at the Si/SiO2 interface. Electrical stresses are applied that mimics long-term device performance. Studies of pre- and post- hot carrier and Fowler-Nordheim electrical stresses are applied, in addition to trench physical parameters variation. Moreover, the n-UMOSFET, under post packaging exhibits Negative Bias Thermal Instabilities, NBTI. The latter behavior is typical of digital p-MOSFET. Upon closer scrutiny, a parasitic P-MOSFET is indeed embedded in the structure of the optimized n-MOSFET. The engineering science of the UMOSFET enables the controlled performance, and is today is the device of choice for the MOS-regions within the IGBTs and Thyristors intermediate and high voltage domain devices. Ostensibly, for silicon power devices a number of research issues remain. On the other hand, wide band-gap semiconductor materials with their high operating temperature, critical electric field, thermal conductivities are the prime materials for power PSDs. Wide band-gap materials led to advancements in terms of low cost, size, weight, and high energy density for PSDs. Finally, as a consequence of the high performance demand for these engineering-feat devices, the architecture is complex and reliability is the main research thrust.