Rice University
Smalley-Curl Institute

Transdisciplinary Symposium III
February 9, 2018
This symposium is invitation-only.
Presentation of research results here does not constitute public disclosure.
The Smalley-Curl Institute (SCI) Annual Transdisciplinary Symposium gives graduate students a forum for presenting on their current research, and complements the larger SCI Summer Research Colloquium held in August.

The emphasis is on honing oral presentation skills, so that only short talks are given, both in a traditional 12-minute conference style, as well as very short 5-minute “lightning” talks.

As with our summer event, we award prizes to the best presentations during each session throughout the day (judged by the students in a “people’s choice” style). These prizes will be designated as Travel Awards, to be used for attending professional meetings.

We encourage visitors to come and hear the latest exciting results of our multi-disciplinary research community. For graduate students, take advantage of this event to get to know the work of your peers and spark ideas for possible collaborations!

Represented departments:

**George R. Brown School of Engineering:** Bioengineering, Chemical and Biomolecular Engineering, Civil and Environmental Engineering, Electrical and Computer Engineering, Materials Science and NanoEngineering, Statistics

**Wiess School of Natural Sciences:** BioSciences, Chemistry, Physics and Astronomy

**Smalley-Curl Institute:** Applied Physics

Naomi J. Halas
*Stanley C. Moore Professor in Electrical and Computer Engineering*
*Professor of Physics and Astronomy*
*Professor of Bioengineering*
*Director, Smalley-Curl Institute*

Stanley C. Moore Professor in Electrical and Computer Engineering
Professor of Physics and Astronomy
Professor of Bioengineering
Director, Smalley-Curl Institute

Alberto Pimpinelli
Faculty Fellow, Materials Science and Nanoengineering
Executive Director, Smalley-Curl Institute

Carol Lively
*Administrator, The Applied Physics Graduate Program, Smalley-Curl Institute*

Michelle Downey
Events Specialist, Smalley-Curl Institute

**Graduate Student Planning Committee:**

Charlotte Flatebo, Applied Physics
Melia Bonomo, Applied Physics
Aswathy Girija, Electrical and Computer Engineering
Jason Guo, Bioengineering
Letitia Chim, Bioengineering

Sudeshna Chatterjee, Chemistry
Martin Bell, Applied Physics
Alena Klindziuk, Applied Physics
Haopei Wang, Chemistry
Tien Tang, Bioengineering
**Program**

8:00 AM  
Arrival, set-up, breakfast and coffee

8:30 AM  
Opening Remarks

8:45 AM  
Faculty Keynote Talk:  
Dr. Mustafa Amin

**MORNING SESSION I**  
Session Chair: Melia Bonomo

9:15 AM  
**M1** Daniel Gonzales  
Whole-Brain Imaging of Spontaneous Sleep-Wake Transitions

**M2** Nicole Thadani  
Applying frustration analysis to predict functional domains in adeno-associated virus capsid assembly and disassembly

**M3** Yan Xu  
Heavy Oil Viscosity Reduction Using Iron(III) Tosylate Hexahydrate — A Kinetic and Temperature-Dependent Study

**M4** Kyle Smith  
Circular Differential Scattering of Plasmonic Pinwheels

**M5** Aswathy Girija  
Sensing of Trace Gases using Infrared Spectroscopy

10:15 AM  
BREAK – VOTE

**MORNING SESSION II**  
Session Chair: Haopei Wang

10:20 AM  
**M6** Sandhya Susarla  
Quaternary two-dimensional (2D) transition metal di-chalcogenides (TMDs) with tunable bandgap

**M7** Bryan Anthonio  
Optical Spectroscopy and Control of Quantum Hall Antiferromagnetism in Graphene

**M8** Charlotte Flatebo  
The effect of complex solvent matrices on the dissolution pathways of gold nanorods

**M9** Bhuvanesh Sundar  
A complex network description of quantum systems

**M10** Oliver Dewey  
Optimization of Processing Parameters in Solution Spun CNT Fibers

**M11** Melia Bonomo  
Predicting influenza H3N2 vaccine effectiveness from evolution of the dominant epitope

10:50 AM  
BREAK - VOTE

**MORNING SESSION III**  
Session Chair: Letitia Chim

11:00 AM  
**M12** Sean Bittner  
Fabrication of 3D-Printed, Multilayered Composite Scaffolds for Osteochondral Tissue Repair

**M13** Sudeshna Chatterjee  
Understanding structural landscape of NMDA receptor gating using single molecule FRET

**M14** Yiyuan Yin  
Charge-assembled Fluorescent Gold Microcapsules As A Chromium (VI) Sensor

**M15** Logan Bishop  
Assessing the effects of adsorption site clustering for chromatographic separations

**M16** Fumiya Katsutani  
Direct Observation of Cross-Polarized Excitons in Aligned and Chirality-Enriched Single-Wall Carbon Nanotubes
12:00 PM BREAK - VOTE
12:10 PM BREAK FOR LUNCH
12:45 PM Faculty Keynote Talk: Engineering Multifunctional Nanoparticles for Disease Therapy
  Dr. Gang Bao
AFTERNOON SESSION I Session Chair: Letitia Chim

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<td>1:15 PM</td>
<td>A17</td>
<td>Hierarchical nacre-mimetic, graphene oxide-boron nitride-polymer composites with multifunctional properties</td>
<td>Sung Hoon Hwang</td>
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<td>A18</td>
<td>Lithium metal batteries by ejecting lithium from carbon nanotubes</td>
<td>Gladys Anahí López Silva</td>
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<td>A19</td>
<td>Heterogeneous Plasmon Induced Dissolution of Single Gold Nanorods</td>
<td>Benjamin Hoener</td>
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<td>A20</td>
<td>2H-1T'Structural Phase Transition In CVD-Grown Monolayer Rhenium-Doped Molybdenum Diselenide</td>
<td>Amey Apte</td>
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<td>A21</td>
<td>Adsorptive Desulfurization of Hydrocarbon Fuels with Zeolites</td>
<td>Priscilla Dias da Silva</td>
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<td>A22</td>
<td>Mimicking MSC Condensation to Promote Cartilage Regeneration</td>
<td>Hannah Pearce</td>
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1:45 PM BREAK - VOTE
AFTERNOON SESSION II Session Chair: Martin Bell

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<td>Laser Cooling Ions in a Neutral Plasma</td>
<td>Thomas Langin</td>
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<td>A24</td>
<td>Poly-albumen: Bio-derived Structural Polymer from Polymerized Egg White</td>
<td>Peter Samora Owuor</td>
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<td>A25</td>
<td>Tailoring the Properties of Single-Wall Carbon Nanotube Samples through Structure-Selective Photochemistry</td>
<td>Yu Zheng</td>
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<td>A26</td>
<td>Grain boundary manipulation in directionally solidified oligocrystals</td>
<td>Logan Ware</td>
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<td>A27</td>
<td>Volumetric spatial mapping of cell metabolism in model tissues with embedded hierarchically branched vascular networks</td>
<td>Ian Kinstlinger</td>
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3:00 PM BREAK - VOTE
AFTERNOON SESSION III Session Chair: Martin Bell

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<tr>
<td>3:15 PM</td>
<td>A28</td>
<td>Multi-scale Geometric Design Principles Applied to 3D Printed Schwartzes</td>
<td>Seyed Sajadi</td>
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<td>A29</td>
<td>Multi-lobed point spread functions of fluorescent emitters on large Ag nanowires: simulation and experiment</td>
<td>Rashad Baiyasi</td>
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<td></td>
<td>A30</td>
<td>The management of gold nanorod synthesis with poly(vinylpyrrolidone) of different molecular weights in minor concentration</td>
<td>Katherinne Requejo</td>
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<td>A31</td>
<td>Metallic Ensemble Size Control in Rh/TiO2Catalysts using CO-Mediated Synthesis</td>
<td>Chelsea Clark</td>
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<td>A32</td>
<td>Novel Deep Learning Techniques for Processing-Structure-Property (P-S-P) Predictions</td>
<td>Prabhas Hundi</td>
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<td>4:00 PM</td>
<td><strong>AFTERNOON SESSION IV</strong></td>
<td>Session Chair: Tien Tang</td>
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<td>4:00 PM</td>
<td><strong>A34</strong> Mai Tran</td>
<td>Going green by going blue: Recycling Li-ion batteries by extracting cobalt using deep eutectic solvents</td>
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<td>4:00 PM</td>
<td><strong>A35</strong> Natsumi Komatsu</td>
<td>Toward Single Crystals of Single-Chirality Single-Wall Carbon Nanotubes</td>
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<td>4:00 PM</td>
<td><strong>A36</strong> Ujjal Bhattacharjee</td>
<td>Nanoscale Thermal Localization in Plasmonic Structures: A Direct Investigation by Photothermal Microscopy</td>
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<td>4:00 PM</td>
<td><strong>A37</strong> Daniel Vecchiolla</td>
<td>High Throughput Foam Generation via Bubble-Bubble Pinch-Off in a Microfluidic Expansion Channel</td>
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<td>4:00 PM</td>
<td><strong>A38</strong> Lauren Taylor</td>
<td>Solution Spun MnO$_2$ Doped Carbon Nanotube Fibers for Sewable Supercapacitors</td>
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<td>4:00 PM</td>
<td><strong>A39</strong> Muqing Ren</td>
<td>Atomic iron-dispersed on nitrogen-doped graphene as the O$_2$ electrode catalysts for rechargeable Li-O$_2$(air) battery</td>
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<td>4:30 PM</td>
<td>BREAK – VOTE</td>
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<tr>
<td>4:35 PM</td>
<td>NETWORKING &amp; RECEPTION</td>
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<td>AWARDS CEREMONY</td>
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<td>5:30 PM</td>
<td>CONCLUSION</td>
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Abstracts - Faculty Keynote Speakers:

**Whispers from the Cosmos**

Dr. Mustafa Amin  
Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA

Ripples in spacetime have recently been detected by aLIGO/Virgo detectors. These spacetime whispers have provided unprecedented information about the final dance of binary neutron stars and blackhole mergers. Along with these spectacular recent discoveries, I will discuss other “likely” (more accurately, things I have worked on) sources of such whispers including: (i) the spacetime dynamics close to the big bang, (ii) exotic compact objects made of dark matter in the contemporary universe.

**Engineering Multifunctional Nanoparticles for Disease Therapy**

Dr. Gang Bao  
Department of Bioengineering, Rice University, Houston, TX 77005, USA

The integration of biomolecular engineering, nanotechnology and biology is expected to produce major breakthroughs in medical diagnostics and therapeutics. Due to the size-compatibility of nano-scale structures with proteins and nucleic acids, the design, synthesis and application of nanoprobes, nanocarriers and nanomachines provide unprecedented opportunities for achieving a better control of biological processes, and drastic improvements in disease detection, therapy, and prevention. Recent advances include the development of multi-functional nanoparticles, nano-structured materials and devices, and engineered nucleases for biological and medical applications.

In this talk I will present the recent development and application of magnetic nanoparticles in my lab, including heat generation by magnetic iron oxide nanoparticles for hyperthermia and nanowarming, nanoparticle-based stem cell targeting, and nanocarriers for drug/gene delivery. The opportunities and challenges in nanobioengineering are also discussed.
Abstracts - Symposium Presenters (listed alphabetically by presenter last name):

**Optical Spectroscopy and Control of Quantum Hall Antiferromagnetism in Graphene**

Bryan Anthonio¹, Yunxiang Liao², Matthew S. Foster², and Junichiro Kono¹²³

¹Department of Electrical & Computer Engineering, Rice University, Houston, Texas, USA
²Department of Physics & Astronomy, Rice University, Houston, Texas, USA
³Department of Materials Science & NanoEngineering, Rice University, Houston, Texas, USA

Modern condensed matter physics research places a strong focus on studying novel phases of matter, especially those of strongly-correlated materials. These materials can exhibit exotic features such as high-temperature superconductivity, metal-insulator phase transitions, and giant magnetoresistance, which occur due to strong interactions between electrons. Recent studies have shown that graphene, a single-layer material composed of carbon atoms arranged in a honeycomb lattice, assumes a strongly-correlated phase in the presence of high magnetic fields. In these conditions, the magnetic field quantizes the electronic states into so-called Landau levels. However, an energy gap opens within the lowest Landau level when the Fermi level is exactly zero. When this occurs, the material transforms from a metal into an insulator. A recent electronic transport measurement suggests that the ground state of this configuration is a quantum Hall antiferromagnet in which the spins of electrons located on neighboring carbon atoms align themselves to become anti-parallel due to strong Coulomb interactions. In this talk, I will describe our current efforts aimed at using optical spectroscopy techniques to probe this energy gap of the lowest Landau level and investigate the nonequilibrium dynamics of this system occurring under the influence of strong electromagnetic perturbations induced by intense optical pulse excitations.

**2H-1T’ Structural Phase Transition In CVD-Grown Monolayer Rhenium-Doped Molybdenum Diselenide**

Amey Apte¹, Vidya Kochat¹, Jordan Hachtel², Hiroyuki Kumazoe³⁴, Aravind Krishnamoorthy⁴, Sandhya Susarla¹, Juan Carlos Idrobo², Fuyuki Shimojo³, Priya Vashishta⁴, Rajiv Kalia⁴, Aiichiro Nakano⁴, Chandra Sekhar Tiwary¹, and Pulickel M. Ajayan¹

¹Department of Materials Science & NanoEngineering, Rice University, Houston, TX, USA
²Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN, USA
³Department of Physics, Kumamoto University, Kumamoto, Japan
⁴Collaboratory for Advanced Computing & Simulations, University of Southern California, Los Angeles, CA, USA

We show coexistence of stable 2H-1T’ phase transition in rhenium-doped 2D MoSe₂.
using chemical vapor. Group VIB transition metal dichalcogenides are MX$_2$-type layered van der Waals compounds (M = Mo/W, X = S/Se/Te) with 2H symmetry resulting in a semiconducting behavior. The 1T/1T' symmetry gives rise to semimetallicity but it is not the ground state; these phases can be stabilized via intercalation of lithium atoms. The 2H-1T' phase transition in Redoped MoSe$_2$ is clearly observed in HAADF-STEM imaging and supplemented by DFT simulations. In addition, we observe emergent magnetic properties in 2D alloys which can be applicable in spintronics.

**Multi-lobed point spread functions of fluorescent emitters on large Ag nanowires: simulation and experiment**

Rashad Baiyasi,¹ Christy Landes,¹,² and Stephan Link¹,²  
¹Department of Electrical & Computer Engineering, Rice University, Houston, TX, USA  
²Department of Chemistry, Rice University, Houston, TX, USA

It has been demonstrated that fluorophores close to large metallic nanowires generate non-standard point spread functions based on the position and orientation of the transition dipole. These complex point spread functions possess between one and four lobes – here we have focused our analysis on two-lobed point spread functions due to the information loss in single lobes and the relative infrequency of four-lobed point spread functions. These two-lobed point spread functions are observed in experimental data wherein stationary fluorophores are excited by surface plasmon polariton propagation along Ag nanowires, and compared to point spread functions from finite-difference time-domain simulations. Simulated point spread functions are used to detect two-lobed point spread functions and reject false multi-lobed point spread functions occurring due to stochastic point spread function positioning. In the future, this extraction of transition dipole orientation from multi-lobed point spread functions can provide further insight into heterogenous surface interactions for such applications as the development of nanocatalysts.

**Nanoscale Thermal Localization in Plasmonic Structures: A Direct Investigation by Photothermal Microscopy**

Ujjal Bhattacharjee,¹ Seyyed Ali Hosseini Jebeli,¹ Wei-Shun Chang,¹ David J. Masiello,² and Stephan Link¹  
¹Department of Chemistry, Rice University, Houston, TX, USA  
²Department of Chemistry, University of Washington, Seattle, WA, USA

The ability to control heat flow and thus, localize temperature in nanoscale has important implications for a wide range of applications from data storage to photothermal therapy. We describe a photothermal microscopy study as direct investigation of temperature distribution under continuous illumination in nanoscale regime. We have fabricated gold nanorod heterodimer on glass substrate with varying gap by electron-beam lithography. Single-particle absorption spectra and dark-field scattering spectra were measured to examine coupling between individual nanorods. Subsequently, how excitation wavelength and polarization and coupling strength in the dimer determine the temperature distribution has been probed. Furthermore, thermal discrete dipole
approximation (T-DDA) simulation with coupled Maxwell–heat diffusion equations has been applied to the dimer systems which illustrates that temperature changes can be both localized and controllably directed within certain component in the plasmon-supporting metal nanoparticle assemblies in agreement of experimental results.

Keywords: single particle absorption, photothermal microscopy, plasmonics, thermal localization, electron beam lithography, gold-nanorod dimer

Assessing the effects of adsorption site clustering for chromatographic separations

Logan D.C. Bishop, Nicholas A. Moringo, Hao Shen, and Christy F. Landes

Department of Chemistry, William Marsh Rice University, Houston, TX, USA

Ion exchange chromatography has become a valuable purification technique in the pharmaceutical industry. While it has proven to be suitable for splitting a simple mixture into its constituent components it often suffers losses in separation resolution in more complex systems, such as proteins. Termed tailing, this loss of separability is attributed to the presence of infrequent long-binding adsorption events that extend the elution time of a small subset of the analyte population. Studying these anomalies at a single molecule level has been performed under the assumption that distinct types of sites exist. Though this heterogeneity is reflective of the nature of packed columns, the possibility of longer binding times because of non-uniform site distribution is rarely considered and has not been fully investigated. We assess the origins of tailing in a single site system where the local density of sites is the source of elongated elution times. This hypothesis is tested by Monte Carlo simulations of a particle’s 1D path through a chromatographic column where adsorption density of sites is variable along the trajectory. Packing is simulated by examining the fluctuation of adsorption probabilities for each step in the column. This work will provide insight into the origins of undesirable tailing effects present in separation systems leading to more robust chromatographic column design.

Fabrication of 3D-Printed, Multilayered Composite Scaffolds for Osteochondral Tissue Repair

Sean M. Bittner, Brandon Smith, Luis Diaz-Gomez, Anthony J. Melchiorri, Antonios G. Mikos

Bioengineering, Rice University, Houston, TX
Center for Engineering Complex Tissues

Osteochondral defects, which have limited endogenous capacity for self-repair, remain a challenge for tissue engineering, as they are highly complex despite having an avascular cartilage region. Previous strategies have been limited by the inability to produce mechanically sufficient articular cartilage as well as failure to mimic the complex interplay between cartilage and subchondral bone found in native tissues. Past work in our laboratory has shown that the
development of heterogeneous scaffolds that address the complexity of the osteochondral unit may offer some solutions to these issues. In the present work, porous, multilayered scaffolds using either a poly(ε-caprolactone) (PCL) or gelatin alginate (Gel) backbone were fabricated via a novel multi-material three-dimensional printing (3DP) system for use in osteochondral defect repair. Composite PCL scaffolds were produced by incorporating nano-hydroxyapatite (nHA) powder to mimic the tissue properties of native subchondral bone. Scaffold characterization displayed the ability to homogeneously incorporate nHA within PCL fibers and that printed constructs maintained good fidelity to the original design. Additionally, heterogeneous pore morphologies were incorporated in an effort to match the native architecture. Finally, multimaterial PCL/nHA/Gel scaffolds were produced to provide a basic design for scaffolds to be used in osteochondral defect repair.

Predicting influenza H3N2 vaccine effectiveness from evolution of the dominant epitope

Melia E Bonomo,1,2 Michael W Deem1,2,3

1Department of Physics and Astronomy, Rice University, Houston, TX, USA
2Center for Theoretical Biological Physics, Rice University, Houston, TX, USA.
3Department of Bioengineering, Rice University, Houston, TX, USA

For the 2016-2017 influenza season, the World Health Organization chose an H3N2 vaccine reference strain that was well-matched to the dominant infecting viruses. Results from conventional ferret models however did not explain why effectiveness of the manufactured vaccine was unusually low, at only 20% for adults aged 18-64. Here we use a novel, reliable measure of antigenic distance between the H3N2 vaccine and circulating virus strains that is based on evolution of the hemagglutinin protein’s dominant epitope, which is the viral site to which an antibody binds. This epitope-based measure originates as an order parameter from our statistical mechanics model of the antibody-mediated response to infection following vaccination. We employ this theoretical method, which has an $r^2 = 0.77$ on 45 years of historical data, to predict how well the administered vaccine protects humans. We identify 19% effectiveness for the H3N2 vaccine due to the introduction of substitutions during egg passaging of the reference strain. This work showcases a robust tool for ensuring optimal reference strain selection and accurately predicting manufactured vaccine effectiveness before the start of future influenza seasons.

Understanding structural landscape of NMDA receptor gating using single molecule FRET

Sudeshna Chatterjee,1 Drew M. Dolino,4 David M. MacLean,4 Logan D.C. Bishop,1 Charlotte Flatebo,1 Vasanthi Jayaraman4 and Christy F. Landes1,2,3

1Department of Chemistry, Rice University, Houston, Texas, USA
2Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA
3Smalley-Curl Institute, Rice University, Houston, Texas, USA
Ionotropic glutamate receptors serve as ion channels in neuronal membrane and are responsible for fast excitatory neurotransmission across neuronal synapses in our central nervous system. N-methyl-D-aspartate receptor (NMDAR) is a unique class of glutamate receptors owing to its structural diversity and availability of a number of binding sites on different domains. Ligands binding at specific domains not only activate/deactivate the ion channel, but also can potentially modulate the activated/deactivated state of the channel, in an allosteric fashion. We present experimental strategies to investigate such gating mechanism of NMDAR ion channels. Single molecule Förster resonance energy transfer (smFRET) has been used as a spectroscopic technique to probe structural landscape of the first transmembrane segment of NMDA receptor under resting and various liganded conditions. The results indicate structurally and energetically distinct states corresponding to each liganded conditions and therefore suggest a gating mechanism at this site. The results from this study are expected to elucidate potential drug target sites on glutamate receptors and therefore contribute to the ever expanding research of targeted neurotherapy.

Metallic Ensemble Size Control in Rh/TiO₂ Catalysts using CO-Mediated Synthesis

Chelsea A. Clark,¹ and Michael S. Wong¹,²,³,⁴

¹Department of Chemical and Biomolecular Engineering, ²Department of Chemistry, ³Department of Materials Science & NanoEngineering, ⁴Department of Civil & Environmental Engineering, Rice University, Houston, TX

Platinum-group metals (PGMs) are widely used as industrial catalysts for many important petrochemical synthesis reactions. In industrial applications, PGM nanoparticles (NPs) are dispersed on a high surface area support to increase the exposed metal surface area and maximize catalyst metal utilization. However, the poor control offered by traditional synthetic methods gives NPs that are inhomogeneous in size and shape. Consequently, only a small fraction of the catalyst surface is exposed to the reactants, significantly impacting material and operational costs. Current methods to precisely synthesize supported PGM catalysts suffer from issues of cost and scalability; thus, there is a need to develop synthetic methodologies which allow for better control over catalyst structure on a molecular level.

This project focuses on developing ligand-mediated wet impregnation techniques to control metallic ensemble size, using Rh/TiO₂ as a model. Our strategy is to kinetically control the nuclearity of 2-dimensional metallic Rh ensembles towards a desired size via the in-situ formation of organometallic rhodium carbonyls on the surface of the support. Our results show significant enhancement of CO chemisorption capacity in the catalysts synthesized using the CO-mediated method over traditional impregnation, and suggest that CO-mediated synthesis can effectively increase the exposed Rh surface area in a tunable manner. Developing further correlations between the primary synthesis variables, including CO partial pressure and contact time, should allow for fine-tuned control over the catalyst structure. CO-mediated synthesis is a
promising strategy for the precise design of catalytic nanomaterials, which will improve the sustainability of chemical processes through increased efficiency.

**Optimization of Processing Parameters in Solution Spun CNT Fibers**

Oliver Dewey,¹ Lauren Taylor,¹ and Matteo Pasquali²

¹Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas, USA
²Department of Chemistry Engineering, Rice University, Houston, Texas, USA

CNTs dissolved in chlorosulfonic acid at high concentrations form a liquid crystalline solution which can be extruded into a non-solvent to form fibers with very high specific electrical conductivity and mechanical strength. To date, optimization of fiber properties has relied largely on improving CNT properties or changing the concentration of CNTs dissolved in the superacid solvent. Such solution spinning is a complex process combining mass and energy transport phenomena, phase changes, and complex fluid flow behavior. Understanding the process parameters which influence CNT fiber properties is necessary for optimizing the production of CNT fibers. Here, we present the study and optimization of several CNT fiber spinning process parameters. This includes the introduction of an air gap, control of the coagulation bath temperature and concentration, and control of spinning direction to leverage density-driven flows. Each of the parameters studied delivers a new way to control the mass transport or fluid flow phenomena that govern fiber quality. This allows for greater process control, offering optimization opportunities not available by changing the CNT material or CNT concentration in the spinning solution. We report optimal operating conditions to produce highly aligned, well-packed CNT fibers with specific conductivity approaching that of copper.

**Adsorptive Desulfurization of Hydrocarbon Fuels with Zeolites**

Priscilla Dias da Silva,¹ Michael S. Wong,¹,²,³,⁴ and Kyriacos Zygourakis¹

¹Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas, USA
²Department of Chemistry, Rice University, Houston, Texas, USA
³Department of Materials Science, Rice University, Houston, Texas, USA
⁴Department of Civil and Environmental Engineering, Rice University, Houston, Texas, USA

This work studies the temperature effect on selective adsorptive desulfurization of liquid hydrocarbon fuels with Cu-Y zeolite under mild temperatures (up to 180°C). The sulfur present in hydrocarbon fuels is harmful to the environment and human health and limits the use of hydrocarbon fuels for remote electricity generation with fuel cells. Adsorptive desulfurization using Cu-Y zeolite has been proposed as an alternative desulfurization process to hydrodesulfurization, which is unable to reach ultra-low sulfur levels and is not feasible for scaled down portable fuel cells. In my work, adsorptive desulfurization is carried out in batch reactors under mild conditions (T<180°C; P<15 bar) and the effect of temperature on desulfurization is studied for temperatures between 30°C and 180°C. Representative fuels were used to generate adsorption isotherms at four temperatures in the specified temperature range in
the presence and absence of aromatic compounds. By performing adsorptive desulfurization at temperatures higher than room temperature, the amount of sulfur adsorbed onto the zeolite increased considerably. Additionally, it was observed that Cu-Y zeolite is capable of removing sulfur above the theoretical limit of 1 atom of a sulfur-containing compound per atom of Cu for the representative fuels. The mechanism of adsorption and competitive behavior of aromatic compounds, naturally occurring in liquid fuel, are determining factors for the implementation of adsorptive desulfurization in complex liquid fuels. This work provides insight on the kinetics of sulfur adsorption by Cu-Y zeolite at temperatures above ambient and suggests potential improvement in the process of reduction of sulfur in liquid fuels.

The effect of complex solvent matrices on the dissolution pathways of gold nanorods

Charlotte Flatebo,¹,² Sean Collins,² Ben Hoener,² Yiyu Cai,² Christy Landes²,³

¹Applied Physics Graduate Program, Rice University, Houston, Texas, USA
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Because of the extreme chemical inert nature of gold as a substrate, applications in biological and electrochemical systems are major focuses of gold nanoparticle research. In the anodic region, gold is an electrooxidant; however, in order to use gold as a modified electrode in biological systems, understanding the stability in the presence of different anions, as well as the potential windows in which the gold maintains its shape and desired reactivity, is of the utmost importance. In this study, we observe the effects of complex solvent matrices of anions on gold nanorods (multifaceted gold nanoparticles). Cyclic voltammetry combined with hyperspectral analysis and correlated SEM shows that introducing a small percentage of a competing oxoanion to a chloride-based electrolyte changes the dissolution pathway of the gold nanorods. Introducing acetate does not increase the maximum potential of dissolution, but does protect the surface of the gold nanorod. Introducing bicarbonate causes an initial blue shift with a red-shift back to the original resonance energy when the particles undergo dissolution. Monobasic phosphate causes a blue shift in the plasmon resonance. Furthermore, even in the presence of a high concentration of chloride ions, both bicarbonate and phosphate protect the gold nanorods from dissolution until high anodic potentials are reached. Understanding this phenomenon provides insight into tuning solvent composition as well as potential ranges to efficiently catalyze reactions at higher anodic potentials.

Sensing of Trace Gases using Infrared Spectroscopy

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Developing ultra-sensitive optical sensors for the real-time sensing and monitoring of
potential greenhouse gases such as methane (CH₄) and ethane (C₂H₆) in the atmosphere, is of great importance in environmental monitoring, atmospheric chemistry and for use in the petrochemical industry. Recent advances of interband cascade lasers (ICL) have played a significant role in the development of compact sensors with high sensitivity and low power consumption. Techniques based on laser absorption spectroscopy for trace gas sensing are advantageous compared to other techniques, as they offer high gas specificity and sensitivity, provide fast response times of <1 s, and permit real-time in-situ measurements. Here, we report the spectroscopic detection and real-time monitoring of CH₄ and C₂H₆ based on tunable diode laser absorption spectroscopy (TDLAS) technique. We demonstrate a mid-infrared ICL-based sensor system for the simultaneous detection of trace levels of CH₄ and C₂H₆ and study the thermal effects of the system over a wide atmospheric range. Detection sensitivities of 17.4 ppbv for CH₄ and 2.4 ppbv for C₂H₆ were obtained from Allan deviation analysis, which validates the stability of the system. This sensor architecture has the merits of significantly reduced size and simultaneous detection of two gases without affecting the selectivity, sensitivity and reliability.

**Whole-Brain Imaging of Spontaneous Sleep-Wake Transitions**

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A central goal in neuroscience is to understand how brain-wide activity governs animal behavior. Sleep, for example, is a nearly universal behavior in the animal kingdom characterized by distinct changes in global brain activity. Moreover, we often take for granted that when asleep, the brain is capable of spontaneously initiating the wake state. The ideal experiment for studying such a complex behavior involves monitoring the activity of every neuron in the animal brain during these spontaneous behavioral transitions. Such an experiment would reveal the individual cells and circuits driving sleep-wake behavioral states. However, in all organisms, monitoring brain-wide activity with cellular resolution during fundamental behaviors remains experimentally challenging, and in many cases impossible. For this reason, the tiny roundworm *Caenorhabditis elegans* is an attractive organism for studying global brain dynamics during basic behaviors like sleep. Their small size, fully-mapped nervous system and transparent bodies allow for every neuron in the worm head to be simultaneously recorded using fluorescent indicators. We recently discovered a behavior in which *C. elegans* confined to a microfluidic environment spontaneously transition from high-activity locomotion into a sleep-like state. To fully take advantage of this unique behavior, we are combining this transition with methods for whole-brain imaging to reveal how the worm brain drives spontaneous sleep-wake transitions.

**Heterogeneous Plasmon Induced Dissolution of Single Gold Nanorods**

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Active photocatalysts are important to reduce energy consumption and lower cost for industrial processes. Visible light excitation of local surface plasmon resonances (LSPR) create high local electric fields around the nanoparticle, generate excited charge carriers, and increase the temperature at the nanoparticle surface, all of which can be used for catalytic applications. However, as there are many beneficial catalytic pathways, plasmon enhanced catalytic mechanisms are not well understood. In this work we study the electrochemical dissolution of gold nanorods (AuNRs) in a NaCl electrolyte with and without plasmon excitation. The AuNR dissolution rate was much greater with plasmon excitation. Wavelength dependent measurements demonstrated that direct longitudinal plasmon excitation was responsible for the dissolution rate increase. Since local surface temperature calculations indicated only a small increase at the experimental excitation power density, plasmon generated excited charge carriers best explain the AuNR dissolution rate increase.

Novel Deep Learning Techniques for Processing-Structure-Property (P-S-P) Predictions

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The 21st century is an exciting age for materials discovery as we see unprecedented investments being made in search of advanced multi-functional materials. A key step for accelerated materials discovery is development of thorough multiscale processing-structure-property (P-S-P) maps. The current day norm for developing these maps is based on ab initio and physics based simulations such as molecular dynamics (MD) which are computationally expensive. In our research, we explore the capabilities of novel deep learning techniques, such as convolutional neural networks (CNNs) and multi-layer perceptrons (MLPs), to make accurate P-S-P predictions using only a fraction of the data and computations when compared to MD. Our case study contains hexagonal boron nitride (h-BN) microstructures damaged by various levels of radiation and temperature, and the objective is to predict the residual strength of the structure based on the final atomic positions of the 11,616 atoms that it contains. Using data from MD, we train a CNN model and an MLP model to make these predictions. Our results show that both the methods make reasonably accurate predictions with R² of over 97% and 92% respectively using only about 20% to 40% of MD simulations for training and validation. The results become more interesting with the application of transfer learning techniques. We show that, the model trained using h-BN data can be adapted for predicting properties of other 2-D materials, such as Graphite, with minimal (< 10%) MD simulations of the new material needed for re-training.

Hierarchical nacre-mimetic, graphene oxide-boron nitride-polymer composites with multifunctional properties
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The continuous miniaturization of electronic devices accompanied by the enhanced power density has rendered heat dissipation a critical process for preventing short-circuit. Consequently, constant efforts have been directed towards developing novel composites with high thermal conductivity and electrical insulation for use as materials for electrical product packaging and as substrates for light emitting diodes. Herein, we introduce the ongoing project on the synthesis of nacre-mimetic, multi-layered film, which is composed of repeating layers of two-dimensional materials, graphene oxide and boron nitride coupled with “soft” polymer, such as chitosan. Graphene oxide exhibits excellent electrical and thermal conductivity, while boron nitride is thermally conductive but electrically insulating. Polymer can provide lubricating effects thereby enhancing the overall toughness while achieving high strength. By coupling them together at various ratios, we are aiming to synthesize a ternary composite with the optimum balance of thermal conductivity, mechanical properties and electrical insulation for use in future electronics. The project will have a diverse impact on electronic devices, energy-related materials, automobile industry and construction industry, where efficient heat dissipation and excellent mechanical properties are critical for long-term performances.

Direct Observation of Cross-Polarized Excitons in Aligned and Chirality-Enriched Single-Wall Carbon Nanotubes

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Semiconducting single-wall carbon nanotubes (SWCNTs) possess rich optical properties arising from one-dimensional excitons with extremely large binding energies. Although much has been understood about the properties of excitons that are active for parallel-polarized light, excitons excited by perpendicular-polarized light have not been explored experimentally. Such “cross-polarized” excitons are predicted to exhibit strong many-body effects due to a subtle interplay of quantum confinement and Coulomb interactions. Here, we have directly observed cross-polarized excitons by investigating the polarization dependence of optical absorption in a film of highly aligned, single-chirality SWCNTs. For parallel polarization, strong $E_{11}$ and $E_{22}$ peaks were observed. As the angle between the polarization of the incident beam and the nanotube alignment direction was increased from 0 to 90°, a new peak ($E_{12}/E_{21}$) appeared and grew in intensity at the expense of the $E_{11}$ and $E_{22}$ peaks. The $E_{12}/E_{21}$ peak was observed at 1.88 eV, which is 660 meV higher than $E_{11}$ and 250 meV lower than $E_{22}$. The integrated intensity of the $E_{12}/E_{21}$ peak observed at 90° was ~10% of that of the $E_{11}$ peak observed at 0°. These results allow us to quantify the individual contributions of electron-hole excitonic binding, self-energy correction to
the band gap, environmental influence, and depolarization effects to the transition energy of the cross-polarized exciton.

Volumetric spatial mapping of cell metabolism in model tissues with embedded hierarchically branched vascular networks

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The elegant and intricate mammalian circulatory system evolved to meet the relentless demand for oxygen in the body's dense, metabolically active tissues. Recapitulating the convoluted structure of the vasculature has been a major challenge in the development of engineered tissue models at physiologically relevant scales. Here, we present novel materials and methodology to fabricate model tissues containing complex branching vascular networks. We demonstrate that powdered carbohydrate formulations can be selectively laser sintered to form self-supporting, water-soluble 3D filament networks, which can be used as templates for vascular networks. By casting cell-laden extracellular matrix around the carbohydrate templates, then dissolving templates in aqueous media, vascular networks of unprecedented complexity can be patterned.

There is broad interest in interrogating the spatial changes in cell function which emerge in response to heterogeneous oxygen transport through patterned vessels. We introduce a scalable method for spatially resolving and quantifying the heterogeneous metabolic activity of dense cell populations in patterned hydrogels. Using this method, we measure characteristic zones of viable HepG2 liver cells that survive surrounding patterned channels. This represents an important preliminary step towards characterizing the effectiveness of particular vascular networks in delivering oxygen to engineered tissues.

Our novel fabrication methodology will enable new studies interrogating the effects of oxygen transport on tissue function and will accelerate progress towards functioning model tissues. Furthermore, the ability to spatially map cell function in hydrogels of arbitrary architecture will facilitate discovery of vascular architectures which best support cell survival and tissue-specific functions.

Toward Single Crystals of Single-Chirality Single-Wall Carbon Nanotubes

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Carbon nanotubes (CNTs) continue to attract significant interest due to their unique structural, mechanical, thermal, optical, and electrical properties. However, to further accelerate the development of CNT devices, two challenging goals – macroscopic alignment and chirality sorting – must be achieved simultaneously. Recently, we have developed a method to fabricate wafer-scale films of highly packed and aligned single-wall carbon nanotubes (SWCNTs) utilizing spontaneous global alignment that occurs during vacuum filtration. Furthermore, by
conducting chirality separation prior to the vacuum filtration process, one can use this method to prepare single-chirality aligned SWCNT films – a step toward single crystals of SWCNTs. To further improve the degree of alignment, we have recently implemented an externally applied electric field in the vacuum filtration process. Using an electric field to align CNTs has been previously proven to be promising as it is non-invasive and potentially scalable. The unique combination of vacuum filtration and electric field application will open the door to the production of large-area single-domain films of highly aligned, densely packed, and single-chirality SWCNTs in a desired direction. Data obtained so far suggest that the alignment direction is indeed controllable by an applied electric field. We will further investigate how the degree of alignment depends on the electric field strength, the frequency of the electric field, the concentration of SWCNTs, and the surfactant of SWCNTs, to fully understand the formation dynamics of an aligned CNT network.

Laser Cooling Ions in a Neutral Plasma

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Laser-cooling ions in Penning and Paul traps and atoms in gaseous clouds has enabled groundbreaking advances in quantum information and quantum-degenerate gases, respectively. Recently, molecules, solids, and mesoscopic quantum systems have been laser cooled. Using an ultracold neutral plasma, created by photoionizing atoms in an ultracold gas, we demonstrate the first laser-cooling of ions in a neutral plasma, achieving temperatures as low as 50 mK (a factor of 4 reduction) after 135 μs of cooling. Laser cooling neutral plasmas is typically challenging due to short plasma lifetimes and/or high temperatures. Ultracold neutral plasmas alleviate these concerns, but high collision rates and strong hydrodynamic forces create an environment for laser cooling that differs significantly from other systems.

A major motivation for laser cooling ions in a neutral plasma is to study transport and collective modes under conditions of strong Coulomb coupling. Strong coupling occurs when the ratio between average potential energy of neighboring ions (PE) and thermal kinetic energy (KE), \( \Gamma = \frac{\text{PE}}{\text{KE}} \), exceeds unity. Standard theoretical tools, such as magneto-hydrodynamics and kinetic theories, fail to describe important plasma properties under these conditions. After laser cooling, we observe \( \Gamma \) for ions as high as 11, the highest recorded in a system of this kind. This approaches values for ions in white dwarf stars (\( \Gamma = 10-200 \)) and cores of Jovian planets (\( \Gamma = 20-50 \)), making laser-cooled plasmas promising models for studying physics relevant to astrophysical systems. Laser cooling also demonstrably retards the plasma expansion, raising the possibility of using light-scattering forces to confine a neutral plasma.

Lithium metal batteries by ejecting lithium from carbon nanotubes

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Thanks to their high energy densities, Lithium-metal batteries are part of the next-generation of energy storage devices expected to facilitate the decarbonization of the energy sector. However, lithium is thermodynamically unstable in organic solvents and the deposition of lithium is often heterogeneous. As a result, Li-metal batteries suffer from the formation of Li-dendrites after repeated charge/discharge cycles, which shortens the life of the battery, causes internal short circuits and lowers Coulombic efficiency. Therefore, identifying techniques to stabilize Lithium metal and control its deposition upon cycling is of tremendous importance for realizing Li-metal batteries in commercial markets. Here, we developed a Li-doped multiwall carbon nanotube interlayer that was used to coat the lithium metal surface. We show that the lithiated carbon nanotubes mediate the lithium plating/stripping and prevent side reactions with the electrolyte or the chemical species formed during cycling, such as lithium polysulfides in Li-S batteries. The protected lithium was tested at high current densities (>2 mAh/cm2), showing good rate capability, long-term cycling stability and a lower polarization voltage (< 40 mV vs Li+/Li). Moreover, the formation of lithium dendrites was suppressed. In addition, the protected lithium was used in a full Li-S battery, showing a long-term stability at different current densities. This work demonstrates that controlling the lithium plating/stripping through mediators is a promising strategy to make possible the commercialization of lithium-metal batteries.

Poly-albumen: Bio-derived Structural Polymer from Polymerized Egg White

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Bio-derived materials could play an important role in future sustainable green and health technologies. This work reports the synthesis of a unique egg white-based bio-derived material showing excellent stiffness and ductility by polymerizing it with primary amine-based chemical compounds to form strong covalent bonds. As shown by both experiments and theoretical simulations, the amine-based molecules introduce strong bonds between amine ends and carboxylic ends of albumen amino acids resulting in an elastic modulus of ~4GPa, fracture strength of ~2MPa and a high ductility of 40%. The distributed and interconnected network of interfaces between the hard albumen and the soft amine compounds gives the structure its unique combination of high stiffness and plasticity. A range of in-situ local and bulk mechanical tests as
well as MD simulations reveal a significant interfacial stretching during deformation and a micro-
crack diversion leading to an increased in ductility and toughness. The structure also shows a self-
stiffening behavior under dynamic loading and strength-induced aging suggesting adaptive
mechanical behavior. This egg white derived material could also be developed for bio-compatible
and bio-medical applications.

**Mimicking MSC Condensation to Promote Cartilage Regeneration**

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Cartilage tissue is avascular and possesses very low cell density. As a result, damage to
cartilage is often irreversible. This damage can result from trauma, injury, or disease. Millions of
people are affected and with an aging population, a long-term solution must be found for cartilage
regeneration. In an effort to mimic *in utero* cartilage formation as a means for regenerating
cartilage, a system of microparticles has been proposed that will not only mimic phenomena seen
during fetal cartilage development, but also act as a factor delivery system to promote cartilage
growth. During human development, an event called “MSC condensation” occurs in which human
mesenchymal stem cells (hMSC’s) condense into aggregates before differentiating into
chondrocytes and laying down the extracellular matrix necessary for cartilage development. Using
a biocompatible gelatin microparticle platform, MSC’s will be covalently bound to the surface of
the microparticles and injected into a cartilage defect site. This will ensure the close cell-cell
contact as seen during MSC condensation, and cartilage promoting factors such as hyaluronic acid
and chondroitin sulfate, natural components of the cartilage extracellular matrix, will also be
encased within gelatin microparticles to promote cartilage regeneration. The system will be tested
*in vitro* for cellularity and glycosaminoglycan content, a product of chondrogenic development, to
determine its efficacy before moving to animal studies. In conclusion, the proposed system shows
much promise for cartilage regeneration by mimicking MSC condensation as seen during
embryonic cartilage development and controlling factor presentation to the cells, all within a
gelatin microparticle platform.

**Atomic iron-dispersed on nitrogen-doped graphene as the O2 electrode
catalysts for rechargeable Li-O2(air) battery**

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Lithium – oxygen (air) battery electrochemical performance is limited by the high
overpotential and low cycling stability. Here we present an atomic iron dispersed on nitrogen
doped graphene material as the O2 (air) cathode catalyst. It has a better performance in lowering
the discharge and charge process overpotential and good cyclic stability in air atmosphere than other nitrogen doped graphene-based catalyst. The preliminary result demonstrates atomic iron doped nitrogen graphene as the promising catalyst for the future Li – O₂ (air) battery.

The management of gold nanorod synthesis with poly(vinylpyrrolidone) of different molecular weights in minor concentration

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Gold nanorods (AuNRs) are anisotropic nanoparticles that have attracted great interest because of their unique optical properties and distinct dimensions that enable applications in sensing, imaging and therapy. Despite several investigations have reported the broad longitudinal surface plasmon resonance (LSPR) band tunability, few of them have focused on the synthesis of small particles in high yield. Here, we report a novel, reproducible and scalable protocol for the seedless synthesis of AuNRs with hydroquinone as weak reducing agent and poly(vinylpyrrolidone) (PVP) as additive. The polymer is introduced to growth solutions during synthesis for 100 mM of surfactant cetyltrimethylammonium bromide (CTAB). By using PVP of different molecular weights (5-360 kDa), the LSPR band is tuned from 850 to 1010 nm as a function of polymer addition time. Also, the original aspect ratio (length/width) is reduced at distinct extents depending on the polymer molecular weight. It was found that PVP accelerates the growth rate of AuNRs by more than two times as the molecular weight increases. However, only the use of low molecular weight PVP such as 10 kDa produces AuNRs in high yield. The interaction of the polymer to the nanorod surface was determined by ATR and XPS analysis. It is suggested that PVP interacts with AuNRs through the oxygen atom of the carbonyl group. Because nanomolar concentration of PVP is utilized, it is expected that the polymer acts less like a reducing agent, as seen in traditional polyol synthesis, but as a templating group to stabilize the growing nanorods.

Multi-scale Geometric Design Principles Applied to 3D Printed Schwartzites

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Schwarzites are 3D porous structures with negative Gaussian curvatures, which forms a rigid foam-like structure with unusual mechanical and electronic properties. We investigated the mechanical behavior of primitive and gyroids structures across different length scales. Macroscale structures (cm size) were 3D printed based on molecular models. Molecular dynamics and finite
elements simulations were also used to gain further understanding on compressive loads and kinetic impact experiments. Our results show that these structures hold great promise as high load bearing and impact resistant materials generated due to a unique layered deformation mechanisms. Easily scalable technique such as 3D printing can be explored for other interesting molecular structures to build innovative engineered materials with tunable mechanical response.

Circular Differential Scattering of Plasmonic Pinwheels

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Plasmonic materials with planar, or 2D, chirality have been of recent interest due to their apparent lack of time-reversal symmetry resulting from their perceived sense of twist being different for opposing incident light directions. Here we investigate single planar chiral plasmonic nanostructures by measuring the differences in scattered light with incident left-handed and right-handed light, known as circular differential scattering (CDS). We study lithographically prepared ‘U’ shaped nanostructures arranged in a rotationally symmetric manner and connected by a common center, which we call pinwheels. We observe that pinwheel nanostructures exhibit strong CDS (>30% signal modulation) when excited with total internal reflection excitation. We investigate the mechanism of CDS within this structure and find the fundamental sub-unit required to produce the CDS signal is a single ‘U’ shaped arm connected to a disk structure and not the hypothesized ‘S’ structure which lacked any observable CDS. We also observe that total internal reflection excitation is required to produce the CDS signal which largely vanishes under normal or oblique incidence. We conclude that the CDS results from asymmetric clockwise and counter-clockwise charge oscillations coupling to free-space scattering with different efficiencies according to their rotation relative to the central disk.

A complex network description of quantum systems

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Network analysis is a powerful technique to characterize the structure of connections between agents in a network. The correlations between particles in a quantum system can be profitably viewed as forming a network, where the strength of an edge in the network connecting two particles measures the magnitude of the correlation between them. We use network analysis to describe and characterize the structure of this network encoded in an archetypal quantum system -- an Ising spin chain in a transverse magnetic field. We demonstrate that even in this
simple quantum many-body system, the encoded network features an emergent complexity. Collective network measures of this complex network give insight into the phase diagram not easily captured by more typical quantities, such as the order parameter or correlation length. For example, the network structure varies with transverse field and temperature.

**Quaternary two-dimensional (2D) transition metal di-chalcogenides (TMDs) with tunable bandgap**

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Alloying/doping in two-dimensional transition metal di-chalcogenides (2D TMD’s) has recently become important due to wide range bandgap tunability. However, till now, only binary/ternary alloys have been synthesized with limited band gap tunability. Increasing the number of components would increase the degree of freedom which can provide more flexibility in tuning the bandgap. Herein, synthesis of quaternary alloys \( \text{Mo}_x\text{W}_{(1-x)}\text{S}_{2y}\text{Se}_{2(1-y)} \) is reported using chemical vapor deposition (CVD). By changing the growth temperature, the composition is tuned, which results in a wide band gap tunability from 1.61 to 1.85 eV. A detailed optical study has been done on these quaternary alloys using low-temperature PL. The experimental results were supported by DFT calculations. With such wide range of flexibility in band gap, these materials could be the future materials for optoelectronics.

**Solution Spun MnO\(_2\) Doped Carbon Nanotube Fibers for Sewable Supercapacitors**

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Wearable electronics have become prevalent in today’s society as health monitors, communication devices, and fitness trackers. However, these devices require an energy source to operate. The ideal energy source should be sewn or woven into clothing so that the device does not inhibit the user. Current fiber shaped devices often use metal wires to ensure adequate transport through the length of the device, but these devices suffer from poor flex fatigue and excess weight. Additionally, graphene and carbon nanotube based devices have low efficiency due to poor electron transport. Here, we demonstrate fiber shaped supercapacitor electrodes developed by solution spinning carbon nanotubes and manganese dioxide in chlorosulfonic acid.
These electrodes not only demonstrate excellent capacitance but also exhibit outstanding conductivity and tensile strength. Furthermore, the solution spinning process is scalable and can produce hundreds of meters of continuous electrode. Thus, the presented supercapacitor is suitable for practical applications.

**Applying frustration analysis to predict functional domains in adeno-associated virus capsid assembly and disassembly**

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Viruses are complex nanomachines that facilitate the delivery of genetic material into cells and promote their own replication through the use of multifunctional proteins that undergo a series of conformational shifts. Adeno-associated virus in particular is a small, relatively simple ssDNA virus utilized in gene therapy that exhibits dynamic structural changes throughout its life cycle, but the capsid domains required for these transitions are unknown. Using the frustratometer, a computational tool that analyzes protein structures using thermodynamic modeling to identify key regions facilitating binding and structural transformation, we sought to predict residues of AAV proteins promoting capsid assembly, disassembly, and thermal stability. We identified candidate residues favoring assembled and disassembled states using the frustratometer, then conducted capsid mutagenesis to quantify the impact of these sites on virus functionality. We show that residues identified by the frustratometer play essential roles in virus assembly, thermal stability, and transduction. This work demonstrates a potential application of the frustratometer (and other tools derived from coarse-grained models) in predicting virus formation and function in silico, elucidating the complex thermodynamics underlying virus metastability and accelerating the process of viral nanotherapeutic design.

**Going green by going blue: Recycling Li-ion batteries by extracting cobalt using deep eutectic solvents**

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Increased demand for Li-ion batteries (LIBs) to power the energy needs of the imminent electrification of the transportation sector has caused price surges in the most expensive part of the battery: the cathode, commonly made of cobalt-rich compounds. At a price tag of up to $800/kWh for this chemistry¹, the cobalt within poses not only an economical risk, but a social and environmental challenge that has instigated efforts to reduce the reliance on cobalt while still maintaining high performance.

In this work, a process to extract and reuse cobalt from LIBs containing lithium cobalt (III) oxide has been developed using deep eutectic solvents (DESs), a “green” alternative to
traditional toxic solvents. DESs are made of two or more Lewis or Brønsted acids and bases that mixed together exhibit a deeply depressed freezing point, and can be made from cheap and potentially renewable materials\textsuperscript{2}. The objective is to sustainably recycle cobalt from LIBs and then repurpose it in other energy applications.

Results show that upon heating, the DES dissolves the cathode material, forming a vibrant aqua-blue solution, indicating the presence of Co\textsuperscript{2+} ions. The solubilized metal can then be extracted through filtration and subsequently electrodeposited. Inductively coupled plasma optical emission spectrometry results show record solubility values for a metal oxide in a DES. Furthermore, usage of recovered cobalt in a supercapacitor and a new LIB cell demonstrates that the recycling can go full-circle, applying sustainable means to a sustainable end—or rather a new beginning.

References

**High Throughput Foam Generation via Bubble-Bubble Pinch-Off in a Microfluidic Expansion Channel**

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Paramount to the optimal design of foam generation systems is the understanding of the complex dynamic interactions that govern bubble breakup. Recent experimental work has demonstrated that close confinement of bubbles can facilitate neighbor-neighbor bubble pinch-off, where the strong interactions of two or more neighboring bubbles break a central elongated bubble. This “structure-induced capillary instability” elucidated the process of bubble breakup in sheared foams and manifested in the discovery of two fundamental pore-level mechanisms of foam generation in porous media. The present work offers a novel microfluidic foam generation system for production of ordered, bi- or tridisperse foams, at capacities exceeding 10,000 daughter bubbles per second, through incorporation of the techniques of geometrically mediated splitting and bubble-bubble breakup. Bubble-bubble pinch-off occurs near the entrance of the expansion region of a wide 1600 µm collection channel. Pinch-off is metronomic at sufficiently large strain rates, assisted by a clear templating effect from the bubbles in the expansion. The relationship between the capillary number, the upstream shear rate, and the size distribution of fragmented bubbles is examined. The mechanism of bubble-bubble pinch-off in an expansion differs from the corresponding neighbor-neighbor pinch-off phenomenon discovered in pore constriction studies. The banded size segregation of fragmented and intact bubbles is largely influenced by the geometry of the channel. The optimal design for the formation of bidisperse and tridisperse foams will also be discussed.

**Grain boundary manipulation in directionally solidified oligocrystals**
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Grain boundaries and grain boundary networks strongly influence the performance of polycrystalline materials. Work over the past three decades has shown that tailoring a material’s grain boundary character distribution can improve a variety of properties, including ductility and corrosion resistance. Still, fabricating polycrystals with optimal grain boundary networks remains an open challenge, partly because there is an incomplete understanding of grain boundary structure-property relationships, and partly because traditional processing strategies offer limited control over the character and location of grain boundaries. As a step towards addressing these challenges we report on a technique for manipulating the grain structure in directionally solidified materials. This processing strategy can be used to fabricate geometrically complex bicrystals for high-throughput investigations on grain boundary structure-property relationships as well as net-shaped grain boundary engineered materials.

Heavy Oil Viscosity Reduction Using Iron(III) Tosylate Hexahydrate — A Kinetic and Temperature-Dependent Study

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Heavy oil is an abundant energy resource but its production remains challenging primarily due to its high viscosity. Thermally enhanced oil recovery in the presence of metal-ligand compounds represents a promising method for viscosity reduction. While catalytic chemistry has been proposed to be responsible for effective viscosity reduction, the interactions between metal-ligand compounds and crude oil components at the molecular level are poorly understood and thus the mechanism remains unknown. Here, we studied heavy oil viscosity reduction in a range of 80 - 295 °C with or without iron(III) tosylate hexahydrate (Fe(pts)₃·6H₂O), and analyzed the reaction products via viscometry, TGA-MS, UV-vis-NIR spectroscopy, GC-MS, SARA measurements, XRF and XPS. It was observed that iron complex increased oil viscosity below 220 °C but started to reduce viscosity at 250 °C, and TGA and UV-vis-NIR data also suggested a complete loss of one pts ligand occurred at 250 °C. These results implied that reaching an activation temperature is required for oil viscosity reduction. We also identified 4-methylbenzenethiol in the post-reaction oils (Fe(pts)₃·6H₂O and ≥ 250 °C) by GC-MS, which is likely converted from the released pts ligand that acts as a deviscosifier. SARA analyses showed noticeable drop in resin fraction and XPS analyses showed the aliphatic sulfur content of resins was reduced after the reaction. Our findings revealed some aspects of the fundamental mechanisms of oil viscosity reduction using metal-ligand compounds. This work expands the knowledge of catalytic chemistry and will aid future designs of metal-ligand compounds for thermally enhanced oil recovery.
Charge-assembled Fluorescent Gold Microcapsules As A Chromium(VI) Sensor

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Fluorescent gold nanoclusters (Au NC) are a promising probe material for selective chemical sensing. However, low quantum yields (QY) and an incomplete understanding of the mechanistic origin of the fluorescence limit their practical implementation. We induced glutathione-capped Au NCs to aggregate within silica-coated microcapsular structures using polymer-salt aggregate (PSA) self-assembly chemistry. Whereas free Au NCs have a QY of ~15% and can detect hexavalent chromium Cr(VI) at concentrations as low as 116 ppb (1 μM as chromate) through fluorescence quenching, the encapsulated NCs have a QY of 29% and can detect Cr(VI) at concentrations as low as 5.8 ppb (0.05 μM as chromate). This limit of detection (LOD) is 15× lower than the US EPA maximum contaminant level for total chromium (Cr(III) and Cr(VI), 100 ppb) in drinking water. Whereas low pH values are needed for Au NCs, no pH adjustment is needed using the encapsulated Au NCs, due to the low-pH conditions inside the capsules. This material may be a general means to detect and quantify Cr(VI) and serve as a basis for a practical ion-sensitive sensor at sub-micromolar concentrations.

In Situ Synthesis of Efficient Water Oxidation Catalysts in Laser-Induced Graphene

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NiFe-based catalysts are highly active for the oxygen evolution reaction (OER) in alkaline electrolytes. These catalysts are generally synthesized by solution-based methods. We present an in situ synthesis method for the NiFe-based OER catalysts through a laser-induced graphene (LIG) assisted process. By loading the metal precursor on a pre-formed LIG surface followed by laser scribing, we synthesized the NiFe/LIG catalysts via a solid phase transition that did not require the utilization of CVD or typical solution-based reactions. The catalysts showed high OER activity...
and durability. The overpotential at 10 mA cm$^{-2}$ is as low as 240 mV with a Tafel slope of 32.8 mV dec$^{-1}$ in 1 M KOH. Additionally, this method worked well on a carbon fiber paper substrate providing a convenient approach for the preparation of free-standing catalytic electrode. This method provides a potential route to the facile synthesis of a variety of catalysts on a conductive surface.

**Tailoring the Properties of Single-Wall Carbon Nanotube Samples through Structure-Selective Photochemistry**

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(The author requested to withhold the abstract from being online.)