Rice University
Smalley-Curl Institute

Transdisciplinary Symposium IV
February 8, 2019

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
Professor of Chemistry
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:

Melia Bonomo, Applied Physics
Thasneem Banu Frousnoon, Chemistry
Anthony Giljum, Applied Physics
Cedric Ginestra, Chemical and Biomolecular Eng
Marjan Majid, Bioengineering
Eric Rice, Civil and Environmental Eng
Joseph Young, Electrical and Computer Eng
Joshua Zhao, Applied Physics

Program

8:00 AM	Arrival, set-up, breakfast and coffee		
8:30 AM	Opening Remarks		
8:45 AM	Faculty Keynote Talk: Dr. Aditya Mohite		Halide perovskites: A new class of semiconductors with emergent properties
	MORNING SESSION I *12-minute talks*		Session Chair: Thasneem Banu Frousnoon
9:15 AM	**M1**	Martin Bell	The Rotating Magnetocaloric Effect as a Mechanism for Natural Magnetosensation
	M2	Amit Jain	Ion-exchange Polymer Coated Electrodes for Membrane Capacitive Deionization and Its Application Beyond Desalination
	M3	Benjamin Clark	Chemical Synthesis of Aluminum Nanocubes
	M4	Carlos Origel	Development of a chromosome-integrated genetic orthogonal network for monitoring the unfolded protein response
	M5	Chayan Dutta	Superresolution (fcsSOFI) Imaging of Porous Polymer Support and Active Control of Protein Dynamics
10:15 AM	BREAK – VOTE		
	MORNING SESSION II *5-minute talks*		Session Chair: TBN
10:20 AM	**M6**	Christopher Sylvester	Developing 3-dimensional vascular co-cultures to model atherosclerotic progression after radiation therapy
	M7	Douglas Walker	Computational Design for Structural Control of Collagen Mimetic Peptides
	M8	Henry Yu	Plate Theory for 2D Crystal Flakes on Curved Surfaces
	M9	Esther Lou	Evaluating the Fate of Antibiotic Resistance in An AnMBR
	M10	Hassan Javed	Efficient Removal of Bisphenol-A by Ultra-High Surface Area Porous Activated Carbon Derived from Asphalt
10:45 AM	BREAK - VOTE		
	MORNING SESSION III *12-minute talks*		Session Chair: Anthony Giljum
11:00 AM	**M11**	Hao Mei	Surface segregation of mixed side-chain bottlebrush polymer additives in thin film blends
	M12	Yu Zheng	Controlled Patterning of Carbon Nanotube Energy Levels by Covalent DNA Functionalization
	M13	Abhinav Verma	Verifiable and Interpretable Machine Learning through Program Synthesis
	M14	Danielle Perdue	Exergetic Relationship between the Thermal Properties of Direct Contact Membrane Distillation
	M15	Sara Nizzero	Unraveling synergistic biological transport barriers for injectable inorganic delivery systems
12:00 PM	BREAK - VOTE		
	BREAK FOR LUNCH		

1:00 PM	Faculty Keynote Talk: Dr. Jacob Robinson		Small, Smart, and Connected: Distributed neurotechnology for regulating physiological states
	AFTERNOON SESSION I *5-minute talks*		Session Chair: Joseph Young
1:30 PM	**A16**	Sakib Hassan	Efficiency Limit of Far- and Near-field Thermophotovoltaic Energy Conversion
	A17	Melia Bonomo	Modularity and Flexibility Quantify Unique Perceptions of Music and Speech in the Human Brain
	A18	Lauren McCarthy	The Observation of Trochoidal Dichroism
	A19	Jordin Metz	Extreme Heating at the Nanoscale
1:50 PM	BREAK - VOTE		
	AFTERNOON SESSION II *12-minute talks*		Session Chair: Melia Bonomo
2:00 PM	**A20**	Sean Bittner	3D Printed Dual Vertical Gradient Scaffolds for Bone and Osteochondral Tissue Engineering
	A21	Weijian Li	Tunable optical properties of 1T-TaS2: a room temperature Charge Density Wave material
	A22	Yilin Li	Energy-harvesting windows utilizing dielectric nanoparticles
	A23	Yiyu Cai	Photoluminescence from single copper nanocubes
	A24	Ian Cone	A Circuit Model for Sequence Learning
3:00 PM	BREAK - VOTE		
	AFTERNOON SESSION III *5-minute talks*		Session Chair: TBN
3:10 PM	**A25**	Thasneem Banu Frousnoon	Completion of characterization of OSCs of Solanum lycopersicum and comparison to metabolomics to understand the site of action of triterpenes in the plant
	A26	Ashleigh Smith McWilliams	Fluorescent Surfactant for Real-Time Visualization and Dynamics Studies of Boron Nitride Nanotubes
	A27	Kedar Joshi	The dynamics of colloidal chain inside a spherical cavity
	A28	Zach LaTurner	Two stage process for the production of single cell protein by purple phototrophic bacteria from food waste
3:35 PM	BREAK – VOTE		
	AFTERNOON SESSION IV *5-minute talks*		Session Chair: TBN
3:45 PM	**A29**	Arash Ahmadivand	Toroidal Dipole-Enhanced Third Harmonic Generation of Deep Ultraviolet Light using Plasmonic Meta-Atoms
	A30	Rashad Baiyasi	Quantitative description of nanorod aggregates in scanning electron microscopy images
	A31	Katherinne Isabel Requejo Roque	High yield synthesis and surface modification of small gold nanoplates
	A32	Carlos de los Reyes	Chemical Decoration of Boron Nitride Nanotubes via Reductive Chemistry

	A33	Pratiksha Dongare	Efficiency Enhancement of Solar Photothermal Processes with Photon Flux Redistribution

4:10 PM BREAK – VOTE

4:15 PM NETWORKING & RECEPTION

5:00 PM AWARDS CEREMONY

5:30 PM CONCLUSION

Abstracts - Faculty Keynote Speakers:

Halide perovskites: A new class of semiconductors with emergent properties

Dr. Aditya Mohite

Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX 77005, USA

Halide (hybrid) perovskites (HaP) have emerged as a new class of semiconductors that truly encompass all the desired physical properties for building optoelectronic and quantum devices such as large tunable band-gaps, large absorption coefficients, long diffusion lengths, low effective mass, good mobility and long radiative lifetimes. In addition, HaPs are solution processed or low-temperature vapor grown semiconductors and are made from earth abundant materials thus making them technologically relevant in terms of cost/performance. As a result, proof-of-concept high efficiency optoelectronic devices such as photovoltaics and LEDs have been fabricated. In fact, photovoltaic efficiencies have sky rocketed to 23% merely in the past five years and are nearly on-par with mono-crystalline Si based solar cells. Such unprecedented progress has attracted tremendous interest among researchers to investigate the structure-function relationship and understand as to what makes Halide hybrid perovskites special?
In my talk, I will attempt to answer some of the key questions and in doing so share the results from our work on HaPs over the past four years in understanding structure induced properties of HaPs. I will also highlight fundamental bottlenecks that exist going forward which present opportunities to create platforms to understand the interplay between light, fields and structure on the properties of perovskite-based materials.

Bio: Aditya Mohite is an Associate Professor in the Department of Chemical and Biomolecular Engineering and directs an energy and optoelectronic devices lab working on understanding structure-function properties in materials with the aim of controlling charge and energy flow across. His research philosophy is applying creative and "out-of-the-box" approaches to solve fundamental scientific bottlenecks and they utilize the knowledge to demonstrate technologically relevant performance in devices that is on par or exceeds the current state-of-the-art devices. *He has published more than 120 peer reviewed papers in journals such as Science, Nature, Nature Materials, Nature Nanotechnology, Nano Letters, ACS Nano, Chemical Society Reviews, Applied Physics Letters and Advanced Materials amongst others. He has also delivered more than 85 invited talks.*

Small, Smart, and Connected: Distributed neurotechnology for regulating physiological states

Dr. Jacob Robinson

Department of Electrical & Computer Engineering; Bioengineering, Rice University, Houston, TX 77005, USA

Technological advances in nanoscale materials and devices are allowing us to manipulate and measure brain activity with unprecedented precision leading to deeper understanding of the brain and improved methods to treat brain disorders. In this talk, I will discuss how emerging nanotechnologies enable tiny distributed devices that can be implanted in the body to sense and actuate neural activity. With these electronic, photonic, and magnetic technologies we expect to develop feedback control systems to help regulate physiological states to more effectively treat and a number of disorders.

Bio: Jacob Robinson is an Assistant Professor in Electrical & Computer Engineering and Bioengineering at Rice University and an Adjunct Assistant Professor in Neuroscience at Baylor College of Medicine. Dr. Robinson earned a B.S. in Physics from UCLA and a Ph. D. in Applied Physics from Cornell. Following his Ph. D., he worked as a postdoctoral fellow in the Chemistry Department at Harvard University. Dr. Robinson joined Rice University in 2012 where he currently works on nanoelectronic, nanophotonic, and nanomagnetic technologies to manipulate and measure brain activity. Dr. Robinson is currently a co-chair of the IEEE Brain Initiative, and the recipient of a Hammill Innovation Award, NSF NeuroNex Innovation Award, DARPA Young Faculty Award, and Materials Today Rising Star Award.

Abstracts - Symposium Presenters (*listed alphabetically by presenter last name*):

Toroidal Dipole-Enhanced Third Harmonic Generation of Deep Ultraviolet Light using Plasmonic Meta-Atoms

Arash Ahmadivand,[⊥,‡] Michael Semmlinger,[†,‡] Liangliang Dong,[#,‡] Burak Gerislioglu,[⊥,‡] Peter Nordlander,[⊥,†,‡] and Naomi J. Halas[*,⊥,†,⊥,‡]

[⊥]Department of Physics and Astronomy, [†]Department of Electrical and Computer Engineering, [#]Department of Chemistry, [‡]Laboratory for Nanophotonics, Rice University, 6100 Main Street, Houston, Texas 77005, United States

The harmonic generation of light with plasmonic and all-dielectric nanostructures has gained much recent interest. This approach is especially promising for short wavelength (i.e. ultraviolet (UV)) generation, where conventional nonlinear crystals reach their limits both in transparency and in their ability to achieve phase-matching between the input and output fields. Here we demonstrate that the third harmonic generation of deep UV light in an indium tin oxide (ITO) film can be substantially enhanced by a metasurface consisting of metallic toroidal meta-atoms covered with an alumina layer for protection against laser induced damage. This approach combines the benefits of the large nonlinear susceptibility of ITO with the unique field enhancement properties of a toroidal metasurface. This ITO-meta-atom combination produces a third harmonic signal at a wavelength of 262 nm that is nominally 5 times larger than that of an ITO film patterned with a conventional hotspot-enhanced plasmonic dimer array. This result demonstrates the potential for toroidal meta-atoms as the active engineered element in a new generation of enhanced nonlinear optical materials and devices.

Quantitative description of nanorod aggregates in scanning electron microscopy images

Rashad Baiyasi[1], Miranda J. Gallagher[2], Qingfeng Zhang[2,3], Stephan Link[1,2,3], Christy F. Landes[1,2,3]

[1]*Department of Electrical and Computer Engineering, Rice University, MS 366, Houston, Texas 77005-1892, United States*

[2]*Department of Chemistry, Rice University, MS 60, Houston, Texas 77005-1892, United States*

[3]*Smalley-Curl Institute, Rice University, Houston, Texas 77005, United States*

Aggregation is a major concern when working with colloidal suspensions of nanoparticles. Despite extensive research into the conditions in which nanoparticle aggregation occurs, little has been reported on the inter-particle structure of the aggregates that do form. We have developed two methods for quantitatively measuring the physical structure of nanoparticle aggregates: an algorithm for segmenting dense aggregates measured with scanning electron microscopy (SEM) and an order parameter for characterizing the side-by-side structure. The segmentation algorithm is an application of the marker-controlled watershed method where the nanoparticle markers are isolated through a series of image-processing steps. We have

successfully segmented individual nanoparticles in aggregates under conditions with dim boundaries and intensity variation that preclude the use of other methods. Segmented SEM images can be used to quickly calculate the side-by-side order of a large number of aggregates. We report on the differences in gold nanorod side-by-side order after induced aggregation with bovine serum albumin and salt (NaCl) Future work will see these methods implemented with an open-source, user-friendly interface to provide quantitative image processing tools for researchers to characterize aggregate structure with high throughput.

The Rotating Magnetocaloric Effect as a Mechanism for Natural Magnetosensation

A. Martin Bell[1,2] and Jacob T. Robinson[2,3,4]
[1]*Applied Physics Program, Rice University, Houston, TX, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston TX, USA*
[3]*Department of Bioengineering, Rice University, Houston TX, USA*
[4]*Department of Neuroscience, Baylor College of Medicine, Houston TX, USA*

Many animals demonstrate the ability to detect and respond to magnetic fields far weaker (~50 microteslas) than those used to stimulate synthetic channels (hundreds of milliteslas). While the existence of a magnetic sense is well-established, the mechanism or mechanisms underlying magnetosensation are not known. We propose a mechanism of magnetosensation based on the magnetocaloric effect, where thermally sensitive ion channels respond to energy generated by the entropy changes resulting from rotation of a magnetically anisotropic material in the presence of a magnetic field. Based on our experimental and computational results, it appears that a magnetocaloric model of magnetosensation could provide a magnetic sense in some animals.

We establish a parameter space for candidate magnetic materials, and outline experiments to distinguish magnetic senses resulting from the magnetocaloric mechanism from those resulting from chemical or magnetomechanical mechanisms. Based on these results, we additionally identify promising directions for the development of improved synthetic magnetosensors for remote magnetic control of excitable cells.

3D Printed Dual Vertical Gradient Scaffolds for Bone and Osteochondral Tissue Engineering

Sean M. Bittner,[1,2,3] Brandon T. Smith,[1,2,3,4] Luis Diaz-Gomez,[1,2,3] Carrigan D. Hudgins,[1,2,3] Anthony J. Melchiorri,[1,2,3] Antonios G. Mikos[1,2,3]
[1]*Department of Bioengineering, Rice University, Houston, TX 77030, USA;*
[2]*Biomaterials Lab, Rice University, Houston, TX 77030, USA;*
[3]*NIH / NIBIB Center for Engineering Complex Tissues, USA;*
[4]*Medical Scientist Training Program, Baylor College of Medicine, Houston, TX, USA;*

Recent developments in 3D printing (3DP) research have led to a variety of scaffold designs and techniques for osteochondral tissue engineering; however, demonstrations of simultaneous incorporation of multiple types of gradients remain uncommon. Herein, we describe the fabrication and mechanical characterization of porous poly(ε-caprolactone) (PCL) and PCL-hydroxyapatite scaffolds with incorporated vertical porosity and ceramic content gradients *via* a multimaterial extrusion 3DP system. Uniaxial compression

testing demonstrated an inverse relationship between porosity and compressive strength for uniform porosity scaffolds, however no differences were observed as a result of ceramic incorporation. All scaffolds demonstrated compressive moduli within the appropriate range for trabecular bone, indicating sufficient mechanical strength for bone and osteochondral tissue engineering. Porosity and dual gradient scaffolds demonstrated compressive properties similar to those of the highest porosity uniform scaffolds, indicating that these properties are more heavily influenced by the weakest section of the gradient. All uniform scaffolds recovered to similar heights after 24-48 hours despite different porosities, while the large-pore sections of gradient scaffolds remained significantly more deformed than all other groups. Micro-CT imaging and porosity analysis demonstrated the ability to incorporate a vertical porosity gradient, which may better simulate such a gradient found in native osteochondral tissues, and the printed scaffolds were shown to have sufficient compressive properties for bone tissue engineering. Moving forward, the technique described here will serve as the template for more complex multimaterial constructs with bioactive cues that better match native tissue physiology and promote tissue regeneration.

Modularity and Flexibility Quantify Unique Perceptions of Music and Speech in the Human Brain

Melia E Bonomo[1,2], Christof Karmonik[3,4,5], J Todd Frazier[3], Michael W Deem[1,2,6]
[1]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[2]*Center for Theoretical Biological Physics, Rice University, Houston, TX, USA*
[3]*Center for Performing Arts Medicine, Houston Methodist Hospital, Houston, TX, USA*
[4]*MRI Core, Houston Methodist Research Institute, Houston, TX, USA*
[5]*Department of Radiology, Weill Cornell Medical College, New York, NY, USA*
[6]*Department of Bioengineering, Rice University, Houston, TX, USA*

There is great interest in quantifying the impact of music on the brain, owing to its therapeutic potential for treating neurological disease or trauma. Modularity and flexibility are two quantifiers of functional brain activity that have been demonstrated to predict the relative performance of subjects on cognitive tasks of varying complexities (Yue et al., 2017, *J Cogn Neurosci* 29:9, pp 1532-46; Ramos-Nuñez et al., 2017, *Front Hum Neurosci* 11, p 420). Modularity measures the degree to which functional activity within a module of brain regions is more highly correlated than activity between modules, and flexibility measures the likelihood that brain regions change their module allegiance. Here, we investigated the relationship between whole-brain network modularity and flexibility while subjects actively listened to a variety of auditory pieces that varied in cultural familiarity and emotivity. Our results suggest that the inverse relationship between modularity and flexibility previously seen in resting-state data (Ramos-Nuñez et al., 2017) remains important during speech perception and becomes less essential during music perception. When comparing the whole-brain network of subjects perceiving culturally unfamiliar music versus emotional speech, there was heightened modularity during the speech, which had a meaning and tone that were both relatively simple to understand, and there was heightened flexibility during the unfamiliar music, which was more complex to process. These novel quantifiers of whole-brain activity pave the way for creating individualized predictions of response to music engagement and tailoring music therapy interventions.

Photoluminescence from single copper nanocubes

Yi-Yu Cai,[1] Sean S. E. Collins,[1] Miranda J. Gallagher,[1] Ujjal Bhattacharjee,[1] Runmin Zhang,[2] Chow Tsz Him,[3] Arash Ahmadivand,[2] Alexander Al-Zubeidi,[1] Behnaz Ostovar,[4]

Jianfang Wang,[3] Peter Nordlander,[2,4,5] Christy F. Landes,[1,4] and Stephan Link[1,4]
[1]*Department of Chemistry, Rice University, Houston, Texas, United States*
[2]*Department of Physics and Astronomy, Rice University, Houston, Texas, United States*
[3]*Department of Physics, The Chinese University of Hong Kong, Hong Kong, P.R. China*
[4]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, United States*
[5]*Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, United States*

Single particle photoluminescence of copper nanocubes (CuNCs) reveals the interband emission channels and decay behavior of hot carriers. The effect of band structure on those processes is demonstrated by comparing with gold nanocubes of similar sizes. PL enhancement from the CuNCs' localized surface plasmon resonance is revealed by the PL linewidth and peak position changes as well as the increased quantum yields with decreased CuNCs sizes. The single particle scattering and absorption spectra of CuNCs show the size dependent plasmonic resonances and interband absorption feature. Our study on the energy absorption and decay, as well as electronic transition proprieties of CuNCs will help the rational design of copper based nanocatalysts.

Chemical Synthesis of Aluminum Nanocubes

Benjamin D. Clark,[1] Christian Jacobson,[1] Minhan Lou,[2] Arzeena Ali,[1] Gang Wu,[3] Luca Bursi,[3] David Renard,[1] Ah-Lim Tsai,[3] Peter Nordlander,[2] and Naomi J. Halas,[1,4]
[1]*Department of Chemistry, Rice University, Houston, Texas, United States*
[2]*Department of Physics & Astronomy, Rice University, Houston, Texas, United States*
[3]*Division of Hematology, Department of Internal Medicine, The University of Texas McGovern Medical School, Houston, Texas, United States*
[4]*Department of Electrical & Computer Engineering, Rice University, Houston, Texas, United States*

We demonstrate the chemical synthesis of single-crystalline Al nanocubes by decomposing AlH_3 with Tebbe's reagent in tetrahydrofuran. The size and shape of the Al nanocubes is controlled by the reaction time and the ratio of AlH_3 to Tebbe's reagent, which together with reaction temperature, establish kinetic control over the formation of Al nanocrystals. Electron paramagnetic resonance spectroscopy indicates Tebbe's reagent is reduced by AlH_3, generating $Ti^{3+}Cp_2H_2AlH$-THF, the active catalyst for the reduction of AlH_3 by hydride oxidation. The formation of an Al-C bond between AlH_3 and the cyclopentadienyl ring of $Ti^{3+}Cp_2H_2AlH$-THF with the loss of H_2 is essential to the growth of Al nanocubes, mediating the formation of cubic super-crystals of atomically precise Al clusters that grow into Al nanocubes provided a sufficient excess of AlH_3. Theoretical calculations reveal that Al nanocubes have extremely high localized electric fields at their corners, making these Al nanocrystals cost-effective Earth-abundant alternatives to noble metal nanoparticles for plasmonics.

A Circuit Model for Sequence Learning

Ian Cone,[1,2] Harel Shouval[1]
[1]*Department of Neurobiology and Anatomy, University of Texas Medical School at Houston, Houston, TX, USA*
[2]*Applied Physics Program, Rice University, Houston, TX, USA*

Temporal interval representation has long been an outstanding question in theoretical neuroscience. Traditional Hebbian learning rules fail for temporal sequences due to the so-called temporal

credit assignment problem, the problem of how an action becomes associated in a Hebbian-like manner with a reward or another action that is distal in time. A promising explanation for this is the idea of competitive LTP and LTD like "eligibility traces". These eligibility traces hold a history of synaptic activity before being converted into changes in synaptic strength upon the presentation of reward. A recent study has found evidence that these eligibility traces indeed exist and are consistent with the theoretically proposed mechanism that can be used to associate distal events. My work extends upon these results, by constructing a biophysically realistic network model that can robustly learn and recall sequences of arbitrary order and duration. This model is designed specifically to account for various experimental observations in visual cortex, but it can also be thought of as a general model for different cortical modalities. The network consists of spiking leaky-integrate-and-fire model neurons placed in a modular architecture designed to mimic cortical microcolumns, with training based on a learning rule with LTP and LTD eligibility traces.

Chemical Decoration of Boron Nitride Nanotubes via Reductive Chemistry

Carlos A. de los Reyes,[1] Kendahl L. Walz Mitra,[1] Ashleigh D. Smith,[1] Sadegh Yazdi,[2] Axel Loredo,[1] Frank J. Frankovsky,[1] Emilie Ringe,[2] Matteo Pasquali,[3] Angel A. Martí[1]

[1]*Chemistry Department, Rice University, Houston, TX, USA.*
[2]*Chemical and Biomolecular Engineering Department, Rice University, Houston, TX, USA.*
[3] *Materials Science and NanoEngineering Department, Rice University, Houston, TX, USA .*

While carbon nanotubes (CNTs) are considered the ultimate building blocks for functional macroscopic materials, they lack some properties for their widespread utilization such as high oxidation stability. Boron nitride nanotubes (BNNTs) could complement such properties: aside from being just as strong as CNTs, they possess a uniform wide bandgap and high thermal and chemical stability. However, because of their chemical inertness it has become a challenge to chemically modify them in order to tune their properties. In this work, we present a straightforward way to modify BNNTs with alkyl chains using Billups-Birch reduction conditions. Post-modified BNNTs were shown to form a chemical bond with the carbon moieties, allowing us to individualize them in organic solvents. Additionally, we prove that the alkyl chains are attached to the outermost wall of the nanotubes and that this modification is reversible allowing for recovery of pristine BNNTs.

Efficiency Enhancement of Solar Photothermal Processes with Photon Flux Redistribution

Pratiksha D. Dongare[1,2,3,4], Alessandro Alabastri[1,2,4], Oara Neumann[1,2], Peter Nordlander[1,2,4,5], and Naomi J. Halas[1,2,4,5,6]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX 77005, USA*
[2]*Laboratory for Nanophotonics, Rice University, Houston, TX 77005, USA*
[3]*Applied Physics Graduate Program, Rice University, Houston, TX 77005, USA*
[4]*Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment (NEWT), Rice University, Houston, TX 77005, USA*
[5]*Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*
[6]*Department of Chemistry, Rice University, Houston, TX 77005, USA*

The increasing fresh water demands of the world have made it inevitable to utilize alternative water sources such as abundant seawater and brackish water. Conventional fuel-based desalination technologies can be expensive, energy intensive, and difficult to deploy in remote regions. Alternative solar energy-based methods usually require bulky light concentrating optics and tracking systems to function efficiently. In this research, we demonstrate scalability and enhanced sunlight intensity utilization for nanophotonics-enabled solar membrane distillation (NESMD). We develop a low-cost time-effective spray coating method capable of coating any size of membrane for NESMD. For a given system size with limited incident solar power we redistribute the photon flux on the light facing membrane surface, taking advantage of the non-linear dependence of the water saturation pressure on temperature and thus light intensity. By the addition of 2" diameter Fresnel lens array covering a 4" × 8" NESMD device, we obtain > 50% improvement in purified water production rate at ambient temperature of 20 ºC with localized flux rates up to ~30 kg/m^2·h. We use finite element method based theoretical modeling to understand the flux enhancement and analyze the effect of ambient temperature, focal spot size, and solar intensity on the water production rate. This study shows how photon flux redistribution can enhance incident light utilization and boost the performance of solar based phase-change processes and photothermal reactions in general, bringing them a step closer to practical applications for remote or underserved households and communities.

Superresolution (fcsSOFI) Imaging of Porous Polymer Support and Active Control of Protein Dynamics

Chayan Dutta[†], Christy F. Landes[†‡§]
†Department of Chemistry, [‡]Department of Electrical and Computer Engineering, and [§]Smalley-Curl Institute, Rice University, Houston, Texas 77251, United States

Abstract: Cross-linked hydrogel nanoparticles made of stimuli-responsive smart polymers have attracted considerable attention in several biomedical technology domains ranging from drug delivery, biosensing, and biomolecule separation and purification. The attraction of stimuli-responsive nanogels is their capacity to spatially and chemically transform when environmental shifts take place, such as pH, temperature and ionic strength changes. These stimuli-driven transformations generate a dynamic heterogeneity of nanogels' physio-chemical properties and are the driving forces behind their underlying surface chemistry. However, a molecular level understanding of the specific interactions of biomolecules, such as proteins, at nanogel surfaces is lacking. Active control over these specific nanogel-biomolecule interactions is necessary for predictive and controlled separation.
Characterizing Nanoscale structure and dynamics under ambient conditions is challenging with traditional techniques, such as AFM. Fluorescence correlation spectroscopy combined with Super-resolution Optical Fluctuation Imaging (fcsSOFI) is ideal to understand the complex dynamic behavior of proteins at the porous polymer surface. In this study, the dynamics of a model protein lysozyme on the nanogel surface and inside the nanogel cavity were investigated using fcsSOFI and single particle tracking. Understanding these complex surface and intra-cavity dynamics of biomolecules will instigate further theoretical and experimental studies of these systems. This will inspire better bottom-up design strategies with other stimuli-responsive polymers for various applications including, but not limited to, separation science and biomedical sciences.

Completion of characterization of OSCs of *Solanum lycopersicum* and comparison to metabolomics to understand the site of action of triterpenes in the plant

Thasneem Banu Frousnoon,[1] and Seiichi P. T. Matsuda[1,2]
[1]*Department of Chemistry, Rice University, Houston, Texas, United States*
[2]*Department of BioSciences, Rice University, Houston, Texas, United States*

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

Efficiency Limit of Far- and Near-field Thermophotovoltaic Energy Conversion

Sakib Hassan,[1] Gururaj V. Naik[1]
[1]*ECE department, RICE University, Houston, Texas, USA*

Thermophotovoltaic (TPV) system is a promising solid-state technology for direct heat-to-electricity conversion. It converts thermal emission from a hot emitter into electric energy by a photovoltaic (PV) converter. In TPV system, the emission profile holds the key for high efficiency energy conversion, which needs to be spectrally matched to the PV cell. However, there is no study on what makes an ideal emission profile, the optimal bandgap of PV cell for a given operating condition, and the efficiency limit for such a system. We will address all these aspects of a TPV energy conversion system in this talk. Our analysis shows that sub-bandgap emission suppression and bandgap emission enhancement are the key parameters for high efficiency operation. A suppression of at least 20 dB and an enhancement of at least 100 is necessary for achieving 60% of Carnot efficiency. Further, we also show that radiative heating of the PV cell from the emitter is also an important factor in the overall optimization of the system. Emission bandwidth less than 0.5 eV and high bandgap PV cell are necessary for minimizing heating. Using realistic properties of materials that make emitters, we show that Mo and W are good choices for near-field emitters.

Ion-exchange Polymer Coated Electrodes for Membrane Capacitive Deionization and Its Application Beyond Desalination

Amit Jain,[1,2] Jun Kim,[2,3] Kuichang Zuo,[2,3] Qilin Li,[2,3] Rafael Verduzco[1,2,4]
[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[2]*NSF Nanosystems Engineering Research Center Nanotechnology-Enabled Water Treatment, Rice University, Houston, TX, USA*
[3]*Civil and Environmental Engineering, Rice University, TX, USA*
[4]*Material Science and Nanoengineering, Rice University, Houston, TX, USA*

Capacitive deionization (CDI) is an energy-efficient water treatment technology that removes ionic contaminants from water by utilizing electric potential between two porous carbon electrodes. Currently,

industrial application of CDI is limited to the desalination of low salinity waters due to its nature of not being able to remove toxic ionic contaminants selectively. In this work we are developing a selective CDI approach to selectively remove ionic contaminants such as scale forming divalent ions, heavy metals other harmful ions. Divalent ions such as calcium and sulfonates, cause scale deposition problems for various industrial operations such as membrane-based desalination systems, oil and gas exploration systems, heat exchangers etc. Similarly, various heavy metals (Cu^{2+}, Pb^{2+}, Hg^{2+} etc.) and other toxic contaminants (Arsenic, Nitrates, Chromium etc.) needs to be removed from various source water for drinking water and waste water treatment and reuse applications. Activated carbon based porous electrodes were prepared using a scalable flow coating technique followed by the deposition of ion-exchange layer on the top of the as prepared electrode. Ion-exchange functional groups are incorporated in these ion-exchange coating layers lead which leads to enhanced desalination performance as well as imparts selectivity towards the removal of the desired contaminants. Our proof of the concept experiments demonstrates good removal selectivity for Ca^{2+}/Na^{+} and SO_4^{2-}/Cl^{-}.

Efficient Removal of Bisphenol-A by Ultra-High Surface Area Porous Activated Carbon Derived from Asphalt

Hassan Javed[1,2], Duy X. Luong[1,2,3], Chang-Gu Lee[1,4], Danning Zhang[1,5], James M. Tour[1,2] and Pedro J.J. Alvarez[1,5*]

[1]*NSF Nanosystems Engineering Research Center for Nanotechnology Enabled Water Treatment (NEWT)*
[2]*Dept. of Chemistry, Rice University, Houston, TX 77005*
[3]*Applied Physics Program, Rice University, 6100 Main Street, Houston, TX, 77005, USA*
[4]*Dept. of Environmental and Safety Engineering, Ajou University, Suwon, South Korea.*
[5]*Dept. of Civil and Environmental Engineering, Rice University, Houston, TX 77005*

The talk will cover our recent work on investigating a novel ultra-high surface area porous activated carbon derived from low cost asphalt (AS) for removal of bisphenol A (BPA), a common endocrine disrupting chemical (EDC) in wastewater and natural waters. Adsorption isotherms, kinetics and thermodynamics of BPA adsorption were determined and benchmarked against commercially purchased Darco G-60 activated carbon (AC). The surface area of AS was found to be 3851 m^2/g, which was 4.7-fold larger than that of AC (i.e., 813 m^2/g). This correlated well with the 4-fold higher maximum BPA adsorption capacity on AS (1113 ± 52 mg/g), and was consistent with the similar surface functionality of AS and AC (determined by Fourier-transform infrared spectroscopy). The maximum BPA adsorption capacity of AS was determined to be the highest among reported carbon materials. BPA adsorption kinetics by both materials was limited by slow intraparticle diffusion into the small mesopores and micropores, which resulted in slightly slower adsorption rate for AS that had a greater proportion of micropores than AC. Thermodynamic analysis corroborated that BPA adsorption was favorable and occurred predominantly through π-π interaction as indicated by Raman spectroscopy. Overall, AS was found to be a highly efficient adsorbent for removal of EDCs for water purification and could be considered for drinking water treatment and wastewater polishing.

The dynamics of colloidal chain inside a spherical cavity

Kedar Joshi,[1] Ziyi Zhu,[1] and Sibani Lisa Biswal[1]

[1]*Department of chemical and biomolecular engineering, Rice University, Houston, USA*

Externally actuated colloidal particles are building blocks for fabricating a variety of anisotropic

shapes. We fabricate wormlike (chain) structures of paramagnetic colloids by connecting them using □-DNA in the presence of an external magnetic field. These chains resemble a structure of different macromolecules like DNA, actin, etc. We use both experimental and computational techniques to study the behavior of these chains under a confined environment. This system mimics many natural phenomena such as DNA packaging, viral insertion, polymer encapsulation, etc. We demonstrate a novel method to build these structures inside a microdroplet. The microdroplet uniformly shrinks which allows us to understand the dynamics of the wormlike chains under a weak as well as strong confinement. Also, this method allows direct observations of conformational preferences and structural changes under the confinement, which will help in deciphering many natural processes.

Two stage process for the production of single cell protein by purple phototrophic bacteria from food waste

Zach LaTurner[1] and Lauren Stadler[1]
[1]*Department of Civil and Environmental Engineering, Rice University, Houston, Washington, United States*

Over one billion tons of food waste is sent to landfills each year where it takes up space and produces greenhouse gases as it decays. Therefore, resource recovery from food waste is an opportune pathway to promote sustainability in our future cities. Microorganisms can consume organic wastes to produce single cell protein (SCP). SCP may then replace current protein sources in livestock feed that are energy intensive and environmentally damaging to produce.

Purple phototrophic bacteria (PPB) have attracted recent attention for SCP production due to their high protein content and favorable amino acid profile. Previous work feeding organic waste to PPB has been hampered by low COD removal efficiencies, resulting in effluent streams unsuitable for direct discharge to the environment. To improve effluent quality in a PPB recovery process, we propose to implement a two-stage process. The first stage, an acid phase anaerobic digester, will break down food waste into volatile fatty acids (VFAs). VFAs have been shown to be an ideal substrate for PPB. The second stage, a PPB enrichment, will consume VFAs and ideally generate an effluent with low COD. In this study, we characterize the performance of a sequencing batch reactor containing an enrichment of PPBs and fed a mixture of VFAs. Previous studies showed that the VFA profile can be controlled by varying operational variables in acid-phase digesters. We examine how the influent profile of VFAs and residence time of the reactor impact the biomass and protein yields of the PPB culture and the effluent quality.

Tunable optical properties of 1T-TaS_2: a room temperature Charge Density Wave material

Weijian Li,[1,2] and Gururaj V. Naik[2]
[1]*Applied Physics Graduate Program, Smalley-Curl Institute, University, 6100 Main Street MS-378, Houston, TX 77005, USA*
[2]*Electrical & Computer Engineering, University, 6100 Main Street MS-378, Houston, TX 77005, USA*

Tunable optical devices are needed for a wide range of applications including imaging, displays, and sensors. Such devices have been demonstrated for several decades using many solid-state materials such semiconductors, polymers and graphene. However, the unavoidable large nonlocal stimulus such as

large charge build-up or high pressure limit their performance in the visible wavelengths for room temperature applications. Here, we report a quasi-2D strongly correlated material exhibiting charge density wave (CDW) order at room temperature, 1T-TaS_2, whose optical properties can be tuned by an in-plane electrical bias that controls the condensation of sliding CDWs at room temperature. We measured the anisotropic dielectric functions of mechanically exfoliated thin films of 1T-TaS_2 and characterized the change in dielectric functions with an in-plane electrical bias and incident light intensity. A maximum refractive index change on the order of 0.1 in the visible range with DC and AC in-plane biases is observed. With light, a maximum refractive index changes of about 0.2 is observed for a moderate incident intensity of 250 mW/cm^{-2}. An optically tunable meta-grating device is proposed where the high intensity illumination shifts the grating's first order diffraction peaks by about 3° and suppresses its intensity by nearly 39% at 550 nm wavelength.

Energy-harvesting windows utilizing dielectric nanoparticles

Yilin Li[1,2] and Rafael Verduzco[1]
[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[2]*Department of Materials Science and Engineering, University of Washington, Seattle, WA, USA*

In this report, proof-of-concept studies were shown for a new type of planar solar concentrator: light scattering based solar concentrator (LSSC). The device consists of a planar optical waveguide doped with dielectric nanoparticles (κ-NPs) that perform light scattering. This design allows photons across nearly the entire solar spectrum to be utilized for optical concentration almost without energy loss. Light scattering Mie theory was used to establish a new approach to describing the size-dependent light scattering capability of κ-NPs towards different portion of sunlight. Two types of LSSCs were fabricated for the application as energy-harvesting windows of building-integrated photovoltaics (BIPV) in the built environment using titanium dioxide κ-NPs. Monte Carlo ray-tracing simulation was used to analyze the system. The results demonstrate several advances in the research of planar solar concentrators, especially compared to luminescent solar concentrators (LSCs). The hazed devices doped with 300-nm κ-NPs to primarily scatter visible light exhibit efficiency up to 4.36% while the transparent devices doped with 500-nm κ-NPs to primarily scatter near-infrared light exhibit efficiency up to 0.95% at a visible transparency of 81%. Artificial neural network was used to optimize the system. Hybrid devices have been developed with the architecture of an LSC stacked on an LSSC. The devices exhibit high efficiency up to 7.58%.

Evaluating the Fate of Antibiotic Resistance in An AnMBR Co-Treating Domestic Wastewater and Livestock Manure

Esther Lou*, Laney Baker*, Adam L. Smith** and Lauren B. Stadler*
*Department of Civil and Environmental Engineering, Rice University
**Sonny Astani Department of Civil and Environmental Engineering, University of Southern California

Anaerobic membrane bioreactors (AnMBRs) show advantages over conventional activated sludge for energy and water recovery from domestic wastewater. Co-management of domestic wastewater with high-strength organic waste streams, such as livestock manure, may improve the system's overall energy balance. Antibiotic resistant bacteria (ARB) and antibiotic resistance genes (ARGs) are an emerging human health risk that warrant attention, particularly in manure co-treatment and agricultural water reuse applications. A limited number of studies have evaluated ARB and ARGs within AnMBRs.

Slower microbial growth rates and other operational parameters may significantly influence horizontal gene transfer and the removal of ARB and ARGs. Here, we evaluate the relationship between organic loading rate, influent antibiotic resistance, and effluent antibiotic resistance in a bench-scale AnMBR treating a mixture of domestic wastewater and livestock manure.

A 5-L AnMBR with ceramic flat sheet membranes (0.1 μm pore size) was fed a mixture of domestic wastewater and tylosin-fed cattle manure slurry. The influent and effluent were sampled regularly for ARG quantification using qPCR. The results showed that the log removal values of *blaOXA-1, blaTEM, ermF, sul2, tetW, ermB* and *ampC* are 1.99, 2.17, 2.37, 2.58, 4.50, 5.23 and 6.65, respectively. Thus, the removal efficiencies of target ARGs are comparable or better than conventional aerobic treatment systems. We also separately quantified ARGs in the cell-associated DNA (caDNA) and cell-free DNA (cfDNA). We found that despite greater concentrations of cfDNA than caDNA in the effluent (9-fold more abundant), the target ARGs were more abundant in caDNA, with the exception of *ermB.* These results highlight the importance of accounting for cfDNA when quantifying ARGs, as it can represent a significant fraction of ARGs discharged by wastewater treatment plants. Ongoing research is focused on assessing ARG removal at incremental organic loading rates.

The Observation of Trochoidal Dichroism

Lauren A. McCarthy,[1,2] Kyle W. Smith,[1,2] Ali Hosseini Jebeli,[2,3] Wei-Shun Chang,[1,2] Stephan Link[1,2,3]

[1]*Department of Chemistry, Rice University, Houston, TX, USA*
[2]*Laboratory for Nanoscale Spectroscopic Imaging, Rice University, Houston, TX, USA*
[3]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*

The sensitivity of matter to light polarization is classically characterized using linear and circular dichroism. Both form ubiquitous optical means of characterizing material geometric properties such as anisotropy and handedness. Recent investigations into polarized confined light, such as evanescent waves formed from total internal reflection, have revealed non-standard light polarizations. Out-of-phase transverse and longitudinal electric field oscillations result in the surprising property of trochoidal, or cartwheeling, field motion which can occur with clockwise and anticlockwise directionality. In this study, we demonstrate matter's sensitivity to the rotational direction of the exciting field and name this property trochoidal dichroism. Trochoidal dichroism was observed in the single particle spectroscopy of a model system composed of capacitively-coupled orthogonal gold nanorods. We find that the resonance wavelength of this system is dependent on the rotational direction of the trochoidal field. This observation constitutes a geometric basis of polarization sensitivity in matter that fundamentally differs from linear and circular dichroism.

Surface segregation of mixed side-chain bottlebrush polymer additives in thin film blends

Hao Mei,[1] Travis Laws,[2] Jiabei Li,[1] Adeline Mah,[3] Tanguy Terlier,[4] David Uhrig,[5] Gila Stein, [2] Rafael Verduzco[1,6]

[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[2]*Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN, USA*
[3]*Materials Science and Engineering Program, University of Houston, Houston, TX, USA*
[4]*Shared Equipment Authority, Rice University, Houston, TX, USA*

[5]*Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, Oak Ridge, TN, USA*
[6]*Materials Science and NanoEngineering, Rice University, Houston, TX, USA*

In blends of linear and branched polymers, the branched polymers spontaneously segregate to interfaces. Prior work has focused primarily on athermal blends. Here, we study thin film blends of mixed side-chain bottlebrush copolymers in a linear matrix of either polystyrene (PS) or polymethyl methacrylate (PMMA). The bottlebrush copolymers are comprised of a polynorbornene backbone grafted with PS and PMMA side-chains. In addition to entropic effects, segregation and phase behavior is governed by enthalpic interactions between the bottlebrush copolymer additives, linear matrix, and film interfaces. We utilize time-of-flight secondary ion mass spectroscopy (ToF-SIMS) to quantify the distribution of bottlebrush copolymers in thin film blends as a function of linear matrix composition, annealing time, and linear matrix molecular weight. Similar to what is observed in athermal film blends, bottlebrush copolymers segregate to film interfaces above a critical linear matrix molecular weight. Segregation is observed in both matrices. Repulsive interactions between the bottlebrush additive and linear matrix result in strong bottlebrush segregation. Segregation is stable under thermal annealing, and a broadening of the mixed phases at the top and bottom of the films is observed. Finally, the choice of linear matrix influences the relative bottlebrush segregation to the top and bottom of the film driven by attractive interactions between the silicon substrate and PMMA chains. This study provides insight into the phase behavior of bottlebrush copolymers mixed with linear polymers. These results show that bottlebrush polymers are versatile additives for tailoring surface and interfacial properties

Extreme Heating at the Nanoscale

Jordin Metz[1,2,3], Pratiksha Dongare[2,3,4,5], Jian Yang[2,3,4], Alessandro Alabastri[2,3,4], Peter Nordlander[2,3,4,6], and Naomi Halas[1,2,3,4,6]
[1]*Department of Chemistry, Rice University, Houston, TX, USA*
[2]*Laboratory for Nanophotonics, Rice University, Houston, TX, USA*
[3]*Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment (NEWT), Rice University, Houston, TX, USA*
[4]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[5]*Applied Physics Graduate Program, Rice University, Houston, TX, USA*
[6]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*

High temperatures are necessary for a range of important chemical reactions, yet require a large energy input that often generates significant greenhouse gases. This project aims to create an array of nanostructures that generate localized extreme temperatures, which could be used for both high temperature chemical reactions and solar steam generation, as an alternative desalination method. The system uses an antenna-reactor combination, specifically with gold bowtie antennas and a gold nanorod reactor. These structures are plasmonic and thus can be synthesized to heat up when irradiated with a particular wavelength of light. The gold bowtie antenna, which looks like two triangles facing each other with a gap in between, scatters the radiation and generates a large electric field in the nano-gap. This effectively amplifies the intensity of the incident laser by ~25 times. The nanorod is placed in this gap, sitting in the hotspot of the near-field enhancement generated by the antenna, and heats up to temperatures of over 1000K, according to simulations. The structures were fabricated using electron-beam lithography and experimental results show the gold nanorod melting to a nanosphere, while the bowtie antennas retain their shape. Temperature measurements are ongoing. Ultimately, this project aims to generate arrays of structures that absorb broadband radiation for use in high temperature chemical reactions and solar steam generation, using light as the energy source to power these important processes.

Unraveling synergistic biological transport barriers for injectable inorganic delivery systems

Sara Nizzero[1,2], Javier Ruiz Ramirez[1], Shreya Goel[1], Mauro Ferrari[1,3,4]
[1]Department of Nanomedicine, Houston Methodist Research Institute, Houston, TX 77030, USA
[2]Materials Science and Nanoengineering, Rice University, Houston, TX 77005, USA
[3]Department of Cell and Developmental Biology, Weill Cornell Medicine, New York, NY, 10065, USA
[4]Department of Medicine, Weill Cornell Medicine, Weill Cornell Medicine, New York, NY, 10065, USA

New understanding in tumor development has highlighted heterogeneity as a major challenge to advanced cancer treatments. An important aspect of systemic heterogeneity is patient physiology, which can be altered by cancer itself, by concurring diseases or conditions, and by previous treatment. Multi-stage delivery strategies have proven the potential of exploiting systemic transport properties connected to physiological parameters to enhance tumor accumulation and directly improve therapeutic efficacy. However, early stage therapeutic development studies are generally conducted on ideal systems with minimal heterogeneity, which may contribute to poor success of clinical translation. In this work, clinically relevant physiological parameters are screened and quantitatively characterized as transport barriers for systemic delivery. Systematic *in vivo* biodistribution studies are conducted to address changes in biodistribution resulting from controlled alteration of specific physiological parameters. Uptake kinetic is characterized through time-resolved analysis, and investigated with an optimized physiologically-based pharmacokinetic (PBPK) model to inform on synergistic, antagonistic, and linear relationships among different parameters. This combined *in vivo* / *in silico* approach enables the quantitative description of mechanistic rules that determine the biodistribution of systemically injected delivery vectors. The framework that emerges from this study opens the way to a new paradigm for personalized adaptive therapy, where therapy can be optimized based on patient-specific physiological profiles.

Development of a chromosome-integrated genetic orthogonal network for monitoring the unfolded protein response

Carlos A. Origel Marmolejo[1], Bhagyashree K. Bachhav[2], Laura Segatori[1,2,3]
[1]BioScience Department, Rice University, Houston, Texas, USA.
[2]Chemical and Biomolecular Engineering Department, Rice University, Houston, Texas, USA.
[3]Bioengineering Department, Rice University, Houston, Texas, USA.

Gene expression regulation in mammalian cells represents the corner stone of the complexity that derives the sophisticated process of translating instructions stored in the genome. More often the study of gene expression signatures and profiles have become the focal point in biological research. Development of novel tools to study gene signaling pathways has been promoted by progress in the field of genome-editing technology and synthetic biology. The objective of this project is to develop a platform technology for monitoring gene expression with high sensitivity and dynamic resolution that captures the complexity of mammalian genetic regulation, thereby providing a reliable tool to profile gene expression signatures. We designed a genetic circuit that implements orthogonal transcription factors and post-translational control elements to monitor endogenous expression of any cellular gene. Integration of mathematical modeling and experimental tests led to the development of a gene reporter platform that can detect changes in gene expression with high sensitivity. To validate the reporter platform, we studied the activation of the unfolded protein response (UPR). The UPR is a cellular mechanism that uses gene regulatory programs to restore protein homeostasis in the endoplasmic reticulum (ER). Loss of protein

homeostasis in the ER is the cellular pathogenesis of a variety of human diseases, primarily neurodegenerative diseases. We implemented the gene reporter platform to study the temporal activation of the UPR signaling pathways upon ER stress stimuli. Results from this project will provide a novel platform technology to monitor cell signaling pathways with superior sensitivity and dynamic resolution.

Exergetic Relationship between the Thermal Properties of Direct Contact Membrane Distillation

Danielle Perdue, Leitao Chen, and Laura Schaefer
Mechanical Engineering Department, Rice University, Houston, Texas, USA

Direct contact membrane distillation (DCMD) is a process that has shown promise within the field of desalination due to its less energy intensive methods and widespread applications. DCMD is a thermally driven microfiltration separation process that operates on the principle of vapor-liquid equilibrium conditions where heat and mass transfer occur simultaneously. Fundamentally, DCMD is based on a porous hydrophobic membrane separating the hot solution (feed) from the cold solution (permeate) where desalinated water condenses. The temperatures at the membrane interface determine the vapor pressure difference across the membrane.

In this work, a direct simulation Monte Carlo analysis is employed to investigate how the exergy of the system relates to other key thermal properties, namely, the temperature polarization coefficient (TPC) and the thermal efficiency (TE), as other parameters are changed, such as feed temperature, flow speed, and membrane porosity. Through molecular simulation, phase equilibrium was reached by calculating the chemical potential at the membrane interface and the entropy of the system was found. Since exergy if a function of entropy, enthalpy, and temperature, the amount of useful work was calculated. Finally, exergy was compared to the TPC and TE as the flow rate and porosity was varied. We demonstrate that with these exergy calculations and the thermal relationship between microscopic and macroscopic scales, a probabilistic range for all parameters will improve future experimental work.

High yield synthesis and surface modification of small gold nanoplates

Katherinne I. Requejo, Anton V. Liopo, and Eugene R. Zubarev
Department of Chemistry, Rice University, Houston, Texas, USA

Gold nanoplates (AuNPs) are two-dimensional anisotropic particles that have received more attention in recent years because of their interesting and unique optical properties that can be tailored for biomedical and sensing applications. At present, few studies have reported the high yield synthesis of AuNPs of different dimensions by the seed-mediated approach. Besides, there is a need to develop reproducible methods to aim for the target applications. Here, we report a novel seeded protocol for the synthesis of monodisperse AuNPs of distinct sizes in high yield with hydroquinone as a weak reducing agent and poly(vinylpyrrolidone) (PVP, 10 kDa) as an additive. At optimal iodide concentrations, the incremental amount of seed solution produces a blue-shift of the surface plasmon resonance (SPR) band indicating a reduction in the edge length (L) of AuNPs from 82 to 52 nm. It was found that as the edge length decreases, the thickness (T) remains constant (13-15 nm) and the aspect ratio (L/T) of AuNPs diminishes from 5.6 to 3.7. Interestingly, the use of nanomolar concentration of PVP during AuNPs growth enhances their monodispersity after purification when compared to controls. Moreover, our reproducible

method enables the formation of AuNPs with long-term shape stability (4 months) in aqueous solution. In addition, surface modification with 11-mercaptoundecyltrimethylammonium bromide (MUTAB) was performed for the biggest aspect ratio AuNPs with and without a polymeric additive. The results indicate that the presence of PVP in MUTAB-coated AuNPs increases the nanoparticle stability as compared to gold nanoplates coated with cetyltrimethylammonium chloride (CTAC) surfactant.

Fluorescent Surfactant for Real-Time Visualization and Dynamics Studies of Boron Nitride Nanotubes

Ashleigh D. Smith McWilliams,[1] Zhao Tang,[2] Selin Ergülen,[1] Carlos A. de los Reyes,[1] Matteo Pasquali,[2] and Angel A. Martí[1]
[1]*Chemistry Department, Rice University, Houston, TX, USA*
[2]*Chemical and Biomolecular Engineering Department, Rice University, Houston, TX, USA*

Boron nitride nanotubes (BNNTs) possess many remarkable properties, such as a uniform wide band gap, excellent thermal conductivity, and superb chemical and thermal stability. However, production of macroscopic BNNT materials has, thus far, not been achieved due to their chemical inertness and poor dispersibility in all solvents. A fundamental understanding of BNNT dynamics in aqueous solution would provide a first step toward utilization of liquid-processing techniques for the production of such macroscopic materials. We developed a novel fluorescent surfactant, in which BNNTs could be individualized and fluorescently tagged. These tagged BNNTs were then visualized by single molecule fluorescence microscopy and their diffusion and bending dynamics were studied for the first time. The rotational and translational diffusions were found to be in agreement with predictions based on a confined, rigid rod undergoing Brownian motion. Additionally, the bending stiffness was found to be too large to measure empirically with current diffraction limits, agreeing with the large persistence length (~7 mm) predicted by theory.

Developing 3-dimensional vascular co-cultures to model atherosclerotic progression after radiation therapy

Christopher B. Sylvester,[1,2] Jun-ichi Abe,[3] and K. Jane Grande-Allen[1]
[1]*Department of Bioengineering, Rice University, Houston, TX, USA*
[2]*Medical Scientist Training Program, Baylor College of Medicine, Houston, TX, USA*
[3]*Department of Cardiology, U.T. M.D. Anderson Cancer Center, Houston, TX, USA*

Radiation exposure, such as that used in cancer treatments, is associated with accelerated cardiovascular disease (CVD), especially atherosclerosis. The mechanisms behind this acceleration are not fully understood, in part because current models are lacking. *In vitro* models that more accurately recapitulate the atherosclerotic environment could improve the study of radiation-induced CVD. Towards this aim, a 3-dimensional (3D) co-culture system was constructed using cross-linkable poly(ethylene glycol) functionalized with the bioactive peptides to allow for cellular adhesion and remodeling. Vascular smooth muscle cells (VSMCs) were encapsulated within the hydrogels, and endothelial cells (ECs) were seeded on top to create an oriented, 3D co-culture. Both cell types adhered to the functionalized hydrogels and expressed phenotypical markers (CD31 and von Willebrand factor for ECs; α-smooth muscle actin for VSMCs). Co-cultures were then irradiated with 0 or 2 Gy of ^{137}Cs γ-rays, comparable to incidental radiation that might be received during therapy. Immunofluorescence demonstrated expression of inflammatory markers (VCAM1 and ICAM1) in ECs. Further, both ECs and VSMCs showed increased

BP53 expression, a marker of DNA breaks after irradiation. Overall, a hydrogel-based co-culture model of atherosclerotic plaque was successfully created. After irradiation, the hydrogel co-cultures replicated some of the key features of radiation-induced CVD such as inflammation and DNA damage. Future work with the developed model will focus on investigating EC-VSMC signaling in the gel, validation with animal models, and incorporating force-generating bioreactors to study how altered mechanics and radiation intersect to increase plaque rupture.

Verifiable and Interpretable Machine Learning through Program Synthesis

Abhinav Verma,[1] and Swarat Chaudhuri[1]
[1]*Computer Science, Rice University, Houston, Texas, USA*

We present a machine learning framework, called Programmatically Interpretable Reinforcement Learning (PIRL), that is designed to generate interpretable and verifiable Artificial Intelligence (AI) agents. PIRL builds on the popular Reinforcement Learning (RL) framework that has been instrumental in the success of many recent AI advancements. Unlike the popular Deep Reinforcement Learning (DRL) paradigm, which represents policies by "black-box" neural networks, PIRL represents policies using a high-level, domain-specific programming language. Such programmatic policies have the benefits of being more easily interpreted than neural networks and being amenable to verification by symbolic approaches used and developed in the Formal Methods community. The generation methods for programmatic policies also provide a mechanism for systematically using domain knowledge for guiding the policy search. The interpretability and verifiability of these policies provides the opportunity to deploy RL based solutions in safety critical environments. We evaluate our approach on the task of learning to drive a simulated car in the TORCS car-racing environment. We demonstrate that our algorithm is able to discover human-readable policies that pass some significant performance bars. We also show that PIRL policies can have smoother trajectories, and can be more easily transferred to environments not encountered during training, than corresponding policies discovered by DRL. This framework opens new avenues for researching connections between the Machine Learning and Formal Methods approaches. Furthermore, by addressing some of the major concerns about the current "black-box" RL methods, this work will advance the applicability and adoption of RL-based solutions to many real-world problems.

Computational Design for Structural Control of Collagen Mimetic Peptides

Douglas R. Walker,[1] Jeffrey D. Hartgerink[1,2]
[1]*Chemistry Department, Rice University, Houston, TX, US*
[2]*Bioengineering Department, Rice University, Houston, TX, US*

Collagen is an integral protein in animals. It is pivotal in the formation of structural features from the aligned structure of bone to the mesh-like network of the extra-cellular matrix. Thus, understanding the molecular structure and the supramolecular interactions in collagen is highly advantageous for developing materials that can mimic these structures. Collagen folds with a PPII helical secondary structure and a triple helical tertiary structure in which three separate protein chains are twisted together. Short "collagen-mimetic peptides" (CMPs) that contain the triplet-repeat pattern emblematic of collagen proteins are a useful model for studying the structure of collagen. This is due to the fact that they fold into the triple helical structure on a reasonable timescale and are water soluble, in contrast with natural collagens. Utilizing our understanding of interactions available to, and found in natural collagen, we have developed methods for controlling the folding of CMPs into specific, composition and register controlled, triple helices. We achieve this by employing specific amino acid substitutions to the canonical collagen

sequence and taking advantage of the associated amino acid pair-wise interactions . These interactions have been compiled as a scoring function that determines the most stable configuration of a given set of peptides. This scoring function has further been employed by a peptide generator which reproducibly generates sets of peptides that will fold into the designed triple helix. This work will be applied to developing CMPs for targeting and binding natural collagens *in vivo*, in addition to designing CMPs to mimic the material properties of natural collagens.

Plate Theory for 2D Crystal Flakes on Curved Surfaces

Henry Yu, Nitant Gupta, Ksenia V. Bets, Boris I. Yakobson
Materials Science & Nanoengineering, Rice University, Houston, TX, 77005

Recent studies have shown great interests and demonstrated the use of substrate topography patterning as a powerful means to engineer strain patterns in 2D materials. These strain patterns can further produce interesting electronic/optical properties in materials, such as band-gap modulations in MoS2 or pseudo-magnetic field in graphene. Indeed, there are existing theories on the elasticity and of layered materials on curved surfaces. However, to our knowledge, these theories assume 1) gradually varying surfaces with small deflections and 2) infinite flake size/absence of edges. Recent experimental works have shown the capability of creating surfaces with sharp features such as cones, pyramids, and toruses, which makes the first assumption invalid. On the other hand, a finite-sized flake on a curved surface is also closer to the conditions of growing crystals, which can lead to very different strain configuration compared to that of an infinite flake. In this work, we present the formally exact equations to calculate the elasticity of 2D crystal flakes on curved surfaces, assuming validity of linear elasticity regime. We also present numerical solutions to optimal strain configurations for graphene, MoS2 and phosphorene flakes on various substrate topographies, with elastic properties parametrized from atomistic simulations. Finally, we calculate the resulting band-gap modulation or pseudo-magnetic field created by these substrate topographies.

Controlled Patterning of Carbon Nanotube Energy Levels by Covalent DNA Functionalization

Yu Zheng,† Sergei M. Bachilo,† and R. Bruce Weisman*,†,‡
†Department of Chemistry and the Smalley-Curl Institute and ‡Department of Materials Science and NanoEngineering, Rice University, 6100 Main Street, Houston, Texas 77005, United States

Single-wall carbon nanotubes exist in a variety of distinct structures. Each is indexed by a pair of integers, (*n*,*m*), and has a well-defined diameter, roll-up (chiral) angle, long-range crystalline order, and uniform electronic properties along its length. Sparse chemical functionalization at random positions on the sidewalls of semiconducting SWCNTs has been shown to introduce local band gap changes that can trap mobile excitons and cause spectrally shifted luminescence. Such chemically modified SWCNTs hold promise as single-photon emitters for applications such as quantum cryptography. To date, however, it has not been possible to control the spatial pattern of covalent functionalization sites or to continuously adjust the band gap modulation. We report here a very simple method for controllable sidewall functionalization of SWCNTs. The nanotubes are first suspended in water by wrapping in ssDNA oligomers. A room temperature covalent reaction between the nanotube surface and guanine nucleotides in the ssDNA coating then proceeds quickly on exposure to singlet oxygen, which is formed through optical excitation of a sensitizer dye. This reaction preserves the SWCNT characteristic short-wave IR fluorescence but causes

spectral red-shifts that depend on the spacing between guanines in the ssDNA oligo. Customized spatial patterns and depths of band gap modulation can thus be inscribed on the nanotube by selecting the templating ssDNA sequence.