

Rice University Smalley-Curl Institute



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SMALLEY-CURL INSTITUTE

**Transdisciplinary Symposium II
February 9, 2017**

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

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Faculty Fellow, Materials Science and Nanoengineering

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Events Specialist, Smalley-Curl Institute

Graduate Student Planning Committee:

John Alred, Materials Science and Nanoengineering

Melia Bonomo, Applied Physics/ Physics

Charlotte Flatebo, Applied Physics/ Chemistry

Loah Stevens, Physics and Astronomy

Mihika Tanzid, Electrical & Computer Engineering

Program

8:00 AM	Arrival, set-up, breakfast and coffee	
8:30 AM	Opening Remarks (Melia Bonomo)	
8:45 AM	Faculty Keynote Talk Dr. Antonios Mikos	Biomaterials for Tissue Engineering
	MORNING SESSION I	Session Chair: John Alred
9:15 AM	M1 Stephen Sanchez	Variance Spectroscopy: A New Bridge between Ensemble and Single-Particle Studies
	M2 Chloe Doiron	Semiconductor Selective Thermal Emitters for the Thermophotovoltaic Applications
	M3 Charlotte Flatebo	Understanding the conformational dynamics of the YfkE trimer using single-molecule Forster Resonance Energy Transfer (smFRET)
	M4 Ya He	Distinct Effects of Inducing or Non-Inducing Auxiliary Substrates on 1,4-Dioxane Biostimulation
	M5 Sung Hoon Hwang	Optimization of the early age strength of CaO-activated fly ash using Taguchi design and microstructural studies
10:15 AM	BREAK – VOTE	
	MORNING SESSION II	Session Chair: Charlotte Flatebo
10:20 AM	M6 Taylor Hernandez	Circular Differential Scattering Studies of Protein Nanorod Aggregate Complexes
	M7 Yilun Li	Three-dimensional Printed Graphene Monolith
	M8 Sonia Parra	A Portable, Lower-Cost High-Resolution Microendoscope (PiHRME) to Screen for Cervical Cancer in Underserved Areas
	M9 Morgan Barnes	Extrusion-Aligned Liquid Crystal Elastomer Fibers
	M10 Melia Bonomo	The CRISPR-Cas Immune System: Fundamentals, Applications, and Future Prospects
	M11 Liyang Lu	4D Compressive Imaging for Hyperspectral Video
10:50 AM	BREAK - VOTE	
	MORNING SESSION III	Session Chair: Melia Bonomo
11:00 AM	M12 Yara Kadria-Vili	Advanced Spectral Analysis for Quantitative Analysis of Single-Walled Carbon Nanotube Samples
	M13 Adam Lauchner	Multicolor Electrochromic Devices Based on Molecular Plasmonics
	M14 Xingcheng Lin	Seeking Out the Functional Mechanism of Influenza Hemagglutinin
	M15 Katherinne Requejo	Accelerating gold nanorod seedless synthesis with nanomolar concentrations of poly(vinylpyrrolidone)
	M16 Tien Tang	Using imaging derived features to predict radiation response
12:00 PM	BREAK - VOTE	
	BREAK FOR LUNCH	
12:45 PM	Faculty Keynote Talk	

Dr. Guru Naik Hot Nanophotonics for Clean Energy

AFTERNOON SESSION I Session Chair: Loah Stevens

1:15 PM	A17	Kimberly Mendoza	Antioxidant Nanocarbon Therapy of Oxidative Stress in Mild Traumatic Brain Injury
	A18	Samantha Paulsen	Design, Fabrication, and Characterization of 3D Printed Microscale Bicuspid Valves
	A19	Dayne Swearer	Aluminum Nanocrystals Decorated with Transition Metal Nanoislands as Antenna-Reactor Nanoparticles for Photocatalysis
	A20	Sangheon Han	Photoacoustic Imaging to Target Specific Cancer Cells Aided by 5nm Molecularly Activated Plasmonic NanoSensors
	A21	Amit Jain	Ion Exchange Polymeric Coatings for Selective Capacitive Deionization
	A22	Yiyu Cai	Mechanism of photoluminescence from plasmonic nanoparticles: Purcell effect enhanced emission from hot carriers

1:45 PM BREAK - VOTE

AFTERNOON SESSION II Session Chair: Mihika Tanzid

2:00 PM	A23	Ching-Wei Lin	In Vivo Detection and Spectral Triangulation of Single-Walled Carbon Nanotubes in Mice
	A24	Julia Vidonish	Pyrolytic Treatment of Soils Remediate Heavy Hydrocarbons and Enhances Fertility
	A25	Carlos de los Reyes	Chemical Decoration of Hexagonal Boron Nitride with Aliphatic Carbon Chains
	A26	Timothy Vu	Study of natural killer cell migration after tumor desensitization by shed NKG2D
	A27	Yu Zheng	Quenching of Single-Walled Carbon Nanotube Fluorescence by Physisorbed Oxygen Reveals Selective ssDNA Affinities

3:00 PM BREAK - VOTE

AFTERNOON SESSION III Session Chair: Melia Bonomo

3:15 PM	A28	Benjamin Hoener	Morphology Dependent Plasmon Shifts by Capacitive Charging
	A29	Barclay Lee	Acquisition of intrinsic cell motility defines natural killer cell maturation from hematopoietic stem cells
	A30	Andrea Miranda	Tailoring development and processing of conjugated polymer binders for use in Si-based Li-ion battery anodes
	A31	Satyajit Rao	Dynamics of stress response in Mycobacterium tuberculosis
	A32	Fengdan Ye	Brain Modularity Mediates the Relation between Task Complexity and Performance

3:40 PM BREAK – VOTE

3:45 PM NETWORKING & RECEPTION

5:00 PM AWARDS CEREMONY

5:30 PM CONCLUSION

Abstracts

Faculty Keynote Speakers:

Biomaterials for Tissue Engineering

Antonios G. Mikos

Department of Bioengineering, Rice University, Houston, Texas

Biomaterial-based strategies for tissue engineering span a vast spectrum from the production of scaffolds tailored with appropriate mechanical properties and degradation kinetics to serve transiently as a bridge to tissue formation to the leverage of biomaterials for the controlled delivery of biological signals to regenerate tissue in specific sites in the body. For example, our laboratory has developed a variety of biodegradable polymers for the controlled delivery of bioactive agents and/or stem cell populations to promote regeneration of tissues such as bone and cartilage. We have also applied engineered culture of cell populations on three-dimensional scaffolds toward the development of biologically active hybrid scaffold/extracellular matrix constructs for regenerative medicine applications as well as testing of anticancer drugs. This talk will present recent examples of biomaterial-based approaches for the development of tissue engineering technologies to meet clinical needs.

Hot Plasmonics: From hot carriers to thermal emitters

Gururaj Naik

Department of Electrical & Computer Engineering, Rice University, Houston, TX

Enhancing light-matter interaction using metal nanostructures is promising for many applications ranging from sensing and medicine to energy and information processing. However, metal nanostructures also enhance light absorption resulting optical loss. Optical losses are not always undesirable, in a particular case of photon upconversion, I will describe how hot carriers created by optical losses in metal may be used to build linear photon upconverters. I will discuss the operation of the first upconverting device working on this principle built from Au/GaN nanostructures. I will conclude my talk with an overview of other fascinating opportunities in plasmonics where optical losses can be turned to our advantage, especially in the context of renewable energy and medicine.

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

Extrusion-Aligned Liquid Crystal Elastomer Fibers

Morgan Barnes,¹ and Rafael Verduzco^{1,2}

¹*Materials Science and NanoEngineering Department, Rice University, Houston, Texas, USA*

²*Chemical and Biomolecular Engineering Department, Rice University, Houston, Texas, USA*

Liquid crystal elastomers (LCEs) are stimuli-responsive shape memory materials that exhibit shape changes when exposed a variety of stimuli such as heat, UV light and electric fields. Potential applications of LCEs include biomedical devices, soft robotics and sensors. However, current synthesis techniques prohibit wide-scale use of LCEs due to current synthesis processes that have limited scalability and primarily 2-dimensional shape changes. This research aims to address these limitations by developing a simple additive manufacturing process to create LCE fiber meshes that elicits complex 3-dimensional shape changes. In preliminary work, we have developed a reaction-extrusion process for the preparation of aligned LCE fibers, which relies on a Michael-addition and UV-initiated thiol-ene reaction that quickly locks in the alignment produced from shear forces. This alignment is critical for the LCE fiber to undergo uni-axial shape changes. Initial alignment of LCE fibers is verified using cross-polarized optical microscopy for a variety of synthesis parameters (i.e. thiol-ene molar ratio, solvent, oligomer size). These results indicate that the thiol-ene chemistry is a good technique for extruding fibers and will be further studied to develop an LCE additive manufacturing process.

The CRISPR-Cas Immune System: Fundamentals, Applications, and Future Prospects

Melia E. Bonomo¹, Michael W. Deem^{1,2}

¹*Department of Physics and Astronomy, Rice University, Houston TX*

²*Department of Bioengineering, Rice University, Houston TX*

The clustered regularly interspaced short palindromic repeats (CRISPR) discovered in prokaryotic genomes in 1987 constitute a novel genetic adaptive immune system. A complex classification system has since then been established for the sizable variety of repeat structures, CRISPR associated (Cas) proteins, target sequence motifs, and functions of these systems. Generally, bacteria and archaea store fragments of invader DNA as “spacers” in a CRISPR locus that can be passed onto their offspring. This genomic memory bank allows these microorganisms to recognize and cleave the DNA of future invaders with the same, or lightly altered, sequences. After it became evident in 2012 that it was possible to harness this mechanism to make precise modifications in a target genome based on a guide sequence, CRISPR-Cas burgeoned as a universal technique in genetic engineering research. While CRISPR work over the past few years has been dominated by gene editing applications, there are still unanswered questions regarding some of the underlying mechanisms of this type of prokaryotic immune system. Here we highlight progress in the key areas of fundamental and applied studies. We additionally emphasize the CRISPR mechanisms that warrant further investigation to understand their associated costs and benefits. Such work will advance applications as well, including efficient

and specific genetic engineering, cell labeling and information storage, and combatting antibiotic resistance.

Mechanism of photoluminescence from plasmonic nanoparticles: Purcell effect enhanced emission from hot carriers

Yi-Yu Cai,¹ Jun Liu,² Eric Sung,¹ Da Huang,¹ Wei-Shun Chang¹, Hui Zhang,² Lawrence J. Tausin,¹ Anneli Hoggard,¹ Mustafa Yorulmaz,¹ Yue Zhang,² Peter Nordlander^{2,3} and Stephan Link^{1,3}

¹*Department of Chemistry, Rice University, Houston, TX, USA*

²*Department of Physics and Astronomy, Rice University, Houston, TX, USA*

³*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*

We proposed that photoluminescence can be used as a probe for hot carriers in plasmonic nanoparticles, because it can be viewed as a Purcell effect enhanced radiative recombination of hot carriers. We correlated the single particle photoluminescence spectra and quantum yield of gold nanorods with five different excitation wavelengths and varied excitation powers experimentally in order to study the effect of hot carrier distributions evolving through interband/intraband transitions and local density of optical states of the particle on photoluminescence. We also performed numerical simulations for photoluminescence spectra based on this mechanism; the simulation results matched experimental spectra well.

Chemical Decoration of Hexagonal Boron Nitride with Aliphatic Carbon Chains

Carlos A. de los Reyes,¹ Ashleigh D. Smith,¹ Kendahl L. Walz-Mitra,¹ and Angel A. Martí¹

¹*Department of Chemistry, Rice University, Houston, TX, USA*

Hexagonal boron nitride (h-BN), structural analog of graphene, possesses unique properties such as uniform wide band gap and high chemical stability. However, this chemical inertness has limited their potential as next generation nanomaterials. From the very few moieties that have been published to chemically attach to the sheets, alkyl grafting examples are even scarcer and require precursor molecules. Herein, bulk h-BN was functionalized with dodecyl chains (fh-BN) using the Billups-Birch conditions, a faster and more straight-forward method. FTIR shows a new pattern of peaks in the 2820-3000 cm⁻¹ assigned to C-H stretching and broadening of the B-N stretching vibration. The modified material exhibits an 8.8% weigh loss in TGA meaning that there is one dodecyl chain per 73 BN units. XPS revealed that only fh-BN presents a significant amount of carbon. Furthermore, such additional features are not present in our control material, which was exposed to the same conditions without the addition of 1-iododecane. The modified material is now more readily dispersible in organic solvents such as hexanes and chloroform than the pristine material. AFM and fluorescence spectroscopy have shown that the dimensions of the functionalized sheets are also larger than the pristine h-BN, showing how the dodecyl chains make larger boron nitride sheets more stable regardless of centrifugation speed.

Semiconductor Selective Thermal Emitters for the Thermophotovoltaic Applications

Chloe F. Doiron^{1,2} and Gururaj V. Naik²

¹*Applied Physics Program, Rice University, Houston, Texas, USA*

²*Electrical and Computer Engineering, Rice University, Houston, Texas, USA*

According to the US Department of Energy, the US industrial sector generates over 1.5 PWh of unrecovered waste heat each year. A significant portion of this waste heat is at reservoir temperatures below 900 K. Thermophotovoltaics (TPV) has the potential to efficiently capture waste heat for electricity generation. TPV relies upon selective emitters, a key component that emits thermal photons in a narrow spectral window which can be efficiently converted to electricity using a photovoltaic (PV) cell. Selective emitters being the bottleneck for higher efficiency, the state-of-the-art high temperature TPV devices barely reach 6% efficiency. For low temperature applications, TPV systems have even lower efficiencies and are thought not useful. But, here we show how proper choice of materials for selective emitters can overcome these limitations and reach efficiencies near 40%. Semiconductors being low loss, tunable, and easy-to-fabricate optical materials, are the best candidates for designing selective thermal emitters. However, their optical properties are not measured at high temperatures. We demonstrate methods to predict the optical properties of semiconductors at high temperatures using carrier scattering models. Understanding the temperature dependence of optical properties allows us to optimize optical losses to enable efficient TPV devices. Additionally, the physical models elucidate material properties and carrier physics to consider when selecting the ideal semiconductor for a specific operating temperature for a selective emitter. With this knowledge, we designed and simulated nanophotonic thermal emitters capable of achieving ideal TPV efficiencies greater than 40% at temperatures below 900 K.

Understanding the conformational dynamics of the YfkE trimer using single-molecule Forster Resonance Energy Transfer (smFRET)

Charlotte Flatebo,^{1,2} Sudeshna Chatterjee,² Logan Bishop,² Yibin Lin,³ Lei Zheng,³
Christy Landes^{2,4}

¹*Applied Physics Graduate Program, Rice University, Houston, Texas, USA*

²*Department of Chemistry, Rice University, Houston, Texas, USA*

³*Department of Biochemistry and Molecular Biology, University of Texas Health Medical School, Houston, Texas, USA*

⁴*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*

Of all the signaling ions regulating biological functions, calcium is the most prevalent and versatile. Although calcium signaling pathways have been extensively studied in eukaryotic organisms, little is known about the role of calcium signaling in bacteria other than limited observations concerning the calcium dependence of movement and growth. The YfkE trimer, a calcium-proton antiporter found in *Bacillus subtilis*, uses a proton gradient to facilitate the

exchange of calcium ions for protons across the cellular membrane; however, the mechanism behind the changes in the conformational states of the trimer has not been fully described. Only the protonated form of the trimer has been crystallized and the proposed mechanism is based on the mechanisms of other transport proteins with similar functionality. Using single-molecule Förster Resonance Energy Transfer (smFRET), we probe the structural changes of the proteins, determining the distribution of states to achieve a bigger picture of the dynamics rather than relying on the single average-values from ensemble measurements such as x-ray crystallography. Elucidating the distribution of states for proteins in calcium depleted, calcium rich and proton rich environments rebukes the previously proposed mechanism. In light of this, we developed an alternative description of the mechanism governing the exchange of calcium ions for protons in the YfkE trimer.

Photoacoustic Imaging to Target Specific Cancer Cells Aided by 5nm Molecularly Activated Plasmonic NanoSensors

Sangheon Han,^{1,2} Richard Bouchard,² and Konstantin Sokolov^{1,2}

¹*Bioengineering, Rice University, Houston, TX*

²*Imaging Physics, The University of Texas MD Anderson Cancer Center, Houston, TX*

Sentinel lymph node biopsy is the gold standard to assess lymphatic metastasis, which is responsible for killing most of cancer patients. However, this technique is invasive in a way that a long-term morbidity is unavoidable and requires a pathologist for the two-weeks awaiting result. Photoacoustic imaging works as irradiation of a tissue with a pulsed laser, differentiating the type of tissues. This combines with ultrasound waves to acquire excellent depth of resolution as well. In addition, this method is a non-invasive and real-time technique without the use of radioactive compounds. We developed a 5nm molecularly activated plasmonic nanosensors (MAPS) to target specific cancer cells for metastatic cancer detection. 5nm MAPS consisted of 5nm spherical gold nanoparticles conjugated with anti-epidermal growth factor receptor (anti-EGFR). Particles smaller than 6 nm are known to achieve renal clearance within hours to days. In cellular level, uptake of 5nm MAPS is mediated by antibody-receptor interaction. This led to aggregation of gold nanoparticle in cells, which creates plasmonic resonance coupling effect. Plasmonic resonance coupling effect from gold nanoparticles is highly detected by photoacoustic imaging. 5nm MAPS showed that development of plasmonic resonance coupling effect at 2 hr under the darkfield imaging and this result applied in the same manner under the photoacoustic imaging. Therefore, the objective of this study was to develop and assess 5nm MAPS in terms of plasmonic resonance coupling as well as photoacoustic signals.

Distinct Effects of Inducing or Non-Inducing Auxiliary Substrates on 1,4-Dioxane Biostimulation

Ya He¹, Yuanyuan Liu², Pedro Alvarez¹, Mengyan Li^{1,3*}

¹*Department of Civil and Environmental Engineering, Rice University*

²*Research Center of Resource Environment and Urban Planning, Changsha University of Science and Technology, Changsha, Hunan, China*

³*Department of Chemistry and Environmental Science, New Jersey Institute of Technology*

Due to its extensive use as the stabilizer, 1,4-dioxane (dioxane) is commonly found at sites impacted by chlorinated solvents, such as 1,1,1-trichloroethane. A microcosm study was conducted to assess two biostimulation strategies (relative to natural attenuation) to bioremediate 1,4-dioxane contamination at a site in west Texas. Dioxane concentrations were relatively low ($< 300 \mu\text{g/L}$), which represents a potential challenge to sustain and induce specific degraders. Thus, biostimulation was attempted with an auxiliary substrate known to induce dioxane-degrading monooxygenases (i.e., tetrahydrofuran [THF]) or with a non-inducing growth substrate (1-butanol [1-BuOH]). Amendment of 1-BuOH (100 mg/L) to microcosms that were not oxygen-limited temporarily enhanced dioxane biodegradation by the indigenous microorganisms. However, this stimulatory effect was not sustained by repeated amendments, which might be attributed to i) the inability of 1-BuOH to induce dioxane-degrading enzymes, ii) curing of catabolic plasmids, iii) metabolic flux dilution and catabolite repression, and iv) increased competition by commensal bacteria that do not degrade dioxane. Experiments with the archetype dioxane degrader *Pseudonocardia dioxanivorans* CB1190 repeatedly amended with 1-BuOH (500 mg/L added weekly for 4 weeks) corroborated the partial curing of catabolic plasmids ($9.5 \pm 7.4\%$ was the plasmid retention ratio) and proliferation of derivative segregants that lost their ability to degrade dioxane. Addition of THF (300 $\mu\text{g/L}$) also had limited benefit due to competitive inhibition; significant dioxane degradation occurred only when the THF concentration decreased below approximately 160 $\mu\text{g/L}$. Overall, these results illustrate the importance of considering the possibility of unintentional hindrance of catabolism associated with the addition of auxiliary carbon sources to bioremediate aquifers impacted with trace concentrations of dioxane.

Circular Differential Scattering Studies of Protein Nanorod Aggregate Complexes

Taylor Hernandez,¹ Kyle W. Smith,¹ and Stephan Link¹

¹*Department of Chemistry, Rice University, Houston, TX, United States*

I propose an experimental approach called circular differential scattering (CDS) which is analogous to ensemble circular dichroism absorption measurements, but measures scattering from single particles rather than absorption from an ensemble. A CDS spectrum can be calculated as the difference between measurements with left and right handed circularly polarized excitation. I hypothesize that proteins adsorbed onto nanoparticles will give some contribution to the CDS signal in these measurements. When nanoparticles are in a protein rich environment, proteins are known to adhere to the surface of the particles. The structural characteristics of proteins on the surface is not known. For the first set of experiments bovine serum albumin (BSA) will be investigated. BSA is structurally similar to human serum albumin, which is the most abundant protein in our blood, and provides a relevant experimental alternative. It has been shown that under certain solution conditions, BSA can induce aggregation of nanorods, which provides a uniquely advantageous platform for these studies because their anisotropy and the random nature of aggregation lead to structures with a high likelihood of being chiral. The chiral structure of the aggregate will generate a local superchiral field, with proteins located on the surface. Plasmon-induced chiral measurements have never

been done on the single particle level, and field enhancements from small inter-particle distances only achievable with chemical preparations will make imaging easier for the pioneer experiment.

Morphology Dependent Plasmon Shifts by Capacitive Charging

**Benjamin S. Hoener¹, Hui Zhang², Thomas S. Heiderscheit¹, Silke R. Kirchner¹,
Agampodi S. De Silva Indrasekara¹, Rashad Baiyasi¹, Yiyu Cai¹, Peter Nordlander^{2,3,4,5},
Stephan Link^{1,2*}, Christy F. Landes^{1,2*}, Wei-Shun Chang^{1*}**

¹*Department of Chemistry, Rice University, Houston, TX, US*

²*Department of Electrical and Computer Engineering, Rice University, Houston, TX, US*

³*Department of Physics and Astronomy, Rice University, Houston, TX, US*

⁴*Applied Physics Program, Rice University, Houston, TX, US*

⁵*Materials Science and Nanoengineering, Rice University, Houston, TX, US*

Plasmonic nanoparticle structures have recently been used as active catalysts for a wide variety of chemical reactions. To incorporate plasmonic particles as catalysts for electrochemical processes, it is important to understand how changing the charge density on a particle affects the plasmonic properties. Previous theoretical predictions demonstrate that plasmon tuning based on charge density is morphology dependent, but the predicted spectral response differs between theories. In this work we compared gold nanorods (AuNRs) and gold nanospheres (AuNSs) of similar surface area to volume ratios to isolate the effect of initial plasmon resonance energy on sensitivity to capacitive charging. We also compared AuNRs of different size and aspect ratio to determine the relationship between initial plasmon resonance wavelength, surface area to volume ratio, and sensitivity to capacitive charging. We conclude that as surface area to volume and initial resonance wavelength are increased, the change in wavelength due to capacitive charging is increased.

Optimization of the early age strength of CaO-activated fly ash using Taguchi design and microstructural studies

Sung Hoon Hwang¹, Vahid Hejazi², Rouzbeh Shahsavari^{1,2,3}

¹*Department of Material Science and Nano Engineering, Rice University, Houston, TX 77005*

²*Department of Civil and Environmental Engineering, Rice University, Houston, TX 77005*

³*The Smalley-Curl Institute, Rice University, Rice University, Houston, TX 77005*

In the light of the cost and safety issues arising from the yet inevitable large dosage of sodium hydroxide and sodium silicate required for activation of fly ash (the byproduct of burning coal in power plants) to be utilized in the design of green construction materials, we propose for the first time, the *cementless*, fly-ash binder composite system, where calcium oxide is applied as the primary activator. The sodium hydroxide and sodium silicate solutions are used as co-activators but in a significantly reduced quantity compared to what is used in conventional methods in the literature. Nanosilica particles (3-5 wt%) are used as additives to further facilitate the strength

development. Via the Taguchi design of experiments, the optimum 7-day compressive strength of 16.18 MPa is achieved, **with** the Ca/Na molar ratio and the amount of nanosilica in the initial system being the two most influential factors on the mechanical strength. The microstructural studies, based on X-ray powder diffraction (XRD), thermogravimetric analysis (TGA-DTA) and scanning electron microscopy energy-dispersive X-ray spectroscopy (SEM-EDS) demonstrate the large contributions of the two factors in the formation of the key products i.e., calcium silicate hydrate, portlandite and $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$.

Ion Exchange Polymeric Coatings for Selective Capacitive Deionization

Amit Jain,¹ Rafael Verduzco,¹ Jun Kim², Qilin Li²

¹*Department Chemical and Biomolecular Engineering, Rice University, Houston, Texas, USA*

²*Department of Civil and Environmental Engineering, Rice University, Houston, Texas, USA*

Capacitive deionization (CDI) is an energy-efficient technology for adsorbing and removing scalants and foulants from water by utilizing electric potential between porous carbon electrodes. Currently, industrial application of CDI is limited to low salinity waters due to the limited absorption capacities of carbon electrodes. However, CDI can potentially be used as a low-cost approach to selectively remove divalent ions from high salinity water. Divalent ions such as sulfonates and carbonates, cause scaling, fouling and thus performance deterioration of membrane-based desalination systems. In this work, we investigated ion-exchange polymer coatings for use in a membrane capacitive deionization (MCDI) process for selective removal of divalent ions. Poly-Vinyl Alcohol (PVA) base polymer was crosslinked and charged using Sulfo-Succinic Acid (SSA) to give a cation exchange type polymer. Experiments on electrodes with as low as 10um thick coating of cation exchange polymer are under progress and will be evaluated on the basis of their selective salt removal efficiency and charge efficiency. Our aim is to tune the crosslink and charge density of the coating layer to maximize the selective removal of divalent ions for high salinity water keeping both salt and charge efficiency high. In future we will be extending this work to sulfonated block copolymers and anion exchange polymers.

Advanced Spectral Analysis for Quantitative Analysis of Single-Walled Carbon Nanotube Samples

Yara Kadria-Vili, Sergei M. Bachilo, and R. Bruce Weisman

Department of Chemistry, Rice University, Houston, TX

Even though single-walled carbon nanotubes (SWCNTs) are of wide interest for various applications, their usage has been hindered by structural heterogeneity. Current synthesis methods produce nanotubes with a broad range of structures having different properties. Efficient analysis methods, such as absorption and emission spectroscopy, are needed to routinely characterize SWCNT sample compositions and guide efforts at structural sorting. However, the reliable interpretation of SWCNT sample spectra is complicated and challenging because of overlapping features from numerous species. We report here two practical approaches that can analyze the spectra of SWCNT samples to provide absolute compositions with a new

level of reliability.

Our first method covers absorption and emission profiles analyses in the short-wave infrared (SWIR) range. This involves two steps: (1) analysis of emission spectra measured with discrete excitation wavelengths to determine the *relative* abundance of semiconducting nanotube species, and (2) analysis of E₁₁ absorption spectra to place the findings from (1) on an *absolute* concentration scale. The method requires information on E₁₁ absorption cross sections and emission profiles, including spectral side bands and their dependence on nanotube structure. We have deduced this information based on studies of single nanotubes and sorted bulk samples.

Our second method covers absorption spectra analysis over the full visible to SWIR range. This analysis includes the visible absorption features, which for each (*n,m*) structure contains the main E₂₂ electronic transition, its exciton-phonon sidebands, and background components. We have deduced peak positions and absorption strengths using photoluminescence excitation profiles (PLEs) measured on sorted samples.

Multicolor Electrochromic Devices Based on Molecular Plasmonics

Adam Lauchner,^{1,4} Grant J. Stec,^{2,4} Yao Cui,^{2,4} Peter Nordlander,^{1,3,4} and Naomi J. Halas^{1,2,3,4}

¹*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*

²*Department of Chemistry, Rice University, Houston, TX, USA*

³*Department of Physics and Astronomy, Rice University, Houston, TX, USA*

⁴*Laboratory for Nanophotonics, Rice University Houston, TX, USA*

Polycyclic aromatic hydrocarbon (PAH) molecules, the hydrogen-terminated, subnanometer scale version of graphene, support plasmon resonances with the addition or removal of a single electron. Typically colorless when neutral, they are transformed into vivid optical absorbers in either their positively or negatively charged states. Here we demonstrate a low-voltage, multistate electrochromic device based on PAH plasmon resonances that can be reversibly switched between nearly colorless (0 V), olive (+4 V), and royal blue (-3.5 V). The device exhibits highly efficient color change compared to electrochromic polymers and metal oxides, lower power consumption than liquid crystals, and is shown to reversibly switch for at least 100 cycles. We also demonstrate the additive property of molecular plasmon resonances in a single-layer device to display a reversible, transparent-to-black device. This work illuminates the potential of PAH molecular plasmonics for the development of color displays and large-area color-changing applications due to their processability and ultralow power consumption.

Acquisition of intrinsic cell motility defines natural killer cell maturation from hematopoietic stem cells

Barclay J. Lee,^{1,2} and Emily M. Mace²

¹*Department of Bioengineering, Rice University, Houston, Texas, USA*

²*Center for Human Immunobiology, Baylor College of Medicine, Houston, Texas, USA*

The contact-dependent factors that regulate human natural killer (NK) cell development remain largely undefined. Two-photon imaging has shown that lymphocytes interact with

stromal cells during *in vivo* migration; however, the migratory behavior of human NK cells is still poorly understood. Previously, we identified a requirement for receptors associated with NK cell terminal maturation in NK cell migration. Therefore, we hypothesized that acquisition of NK cell migration is correlated with cell maturation. To test this hypothesis, we performed long-term continuous live-cell imaging and image analysis of NK cells undergoing *in vitro* development. We observed that NK cell acquired increasing motility during maturation. Tracking of individual cells showed that mean speed and displacement increased steadily as time progressed. At early time points, cells were primarily stationary/subdiffusive, whereas cells showed increasingly directed motility with developmental progression. Despite this, a subset of stationary cells remained and as a result, greater heterogeneity of speed and displacement was observed at later time points. Fluorescence-activated cell sorting (FACS) on multiple developmental markers confirmed that cells exhibited progressive maturation each week. Our data suggests that factors controlling NK cell motility, such as CD56 or CD62L signaling, may play a role in NK cell development. In addition, other surface markers that we observed were acquired during NK cell development, such as CD94 or CD117, may be involved in cell migration as well.

Three-dimensional Printed Graphene Monolith

Yilun Li,¹ Junwei Sha,^{1,2} and James M. Tour^{1,2,3,4}

¹*Department of Chemistry,* ³*The NanoCarbon Center,* ⁴*Department of Materials Science and NanoEngineering, Rice University, 6100 Main Street, Houston, Texas 77005, United States*

²*Collaborative Innovation Center of Chemical Science and Engineering, Tianjin 300350, China*

A simulated powder-bed three-dimensional (3D) printing method for *in-situ* synthesis of free-standing 3D graphene monoliths (GMs) was successfully developed by manually feeding the precursor of Ni/sucrose hybrid powders, and a commercial CO₂ laser was used to convert the hybrid powders into the 3D GMs. Specifically, the sucrose acted as a solid carbon source, and the sintered Ni scaffolds acted as a catalyst and template for graphene growth. This method, which combines powder metallurgy templates method, chemical vapor deposition (CVD), as well as 3D printing technique, is simple and efficient, and enables directly *in-situ* 3D printing GMs with no high-temperature furnace employed and no longtime growth process required. The 3D printed GMs show high porosity of ~99.3%, low density of ~0.015 g cm⁻³, high quality, and multi-layered graphene features, presenting a comparable electrical conductivity of ~8.7 S cm⁻¹, remarkable storage modulus of ~11 kPa, as well as high room temperature damping capacity of ~0.06. These exciting properties of 3D printed GMs indicate good potential applications in fields requiring devisable rapid manufacturing of 3D carbon materials, energy storage devices, damping materials, and sound absorption.

***In Vivo* Detection and Spectral Triangulation of Single-Walled Carbon Nanotubes in Mice**

Ching-Wei Lin,¹ Hailing Yang,³ Sergei M. Bachilo,¹ Robert C. Bast,³
Kathleen M. Beckingham,² and R. Bruce Weisman¹

¹*Department of Chemistry and the Smalley-Curl institute, Rice University, Houston, TX*

²*Department of Biosciences, Rice University, Houston, TX*

³*Department of Experimental Therapeutics, the University of Texas M.D. Anderson Cancer Center, Houston, TX*

Single-walled carbon nanotubes (SWCNTs) hold promise for novel diagnostic and therapeutic medical applications, but methods are required for detecting them at trace concentrations inside tissues. We are developing advanced optical methods for nanotube detection based on their characteristic intrinsic fluorescence at short-wave infrared (SWIR) wavelengths (850-1600 nm). SWIR has the advantages of lower scattering and autofluorescence backgrounds in biological tissues than visible light. However, non-invasive detection of SWCNTs deep in tissues is still challenging because photons are strongly scattered within one millimeter. Hence, fluorescence images based on light reaching the specimen surface are very weak and diffuse. We recently introduced a 3D localization technique called Spectral Triangulation and implemented it using our home-built SWCNT scanner with photon counting detection and state-of-the-art sensitivity. This approach can detect very small amounts of SWCNTs located many millimeters deep inside phantom (artificial) tissues, and deduce the source location to high precision. Here we report recent refinements to our apparatus and methods. We also demonstrate the non-invasive observation of sub-microgram quantities of SWCNTs inside the ovaries of living mice. These results represent a significant step toward a new diagnostic method for detecting cancerous tumors using antibody-targeted SWCNTs.

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Seeking Out the Functional Mechanism of Influenza Hemagglutinin

Xingcheng Lin,^{1,2} Nathaniel R. Eddy,^{1,2} Jeffrey K. Noel,^{1,2} Qinghua Wang,³ Jianpeng Ma,³ and José N. Onuchic^{1,2}

¹*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*

²*Center for Theoretical Biological Physics, Houston, Texas, USA*

³*Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, Texas, USA*

Influenza Hemagglutinin (HA), a membrane surface glycoprotein critical for the infection of flu viruses, has been the target of most flu vaccines in the past years. Previously, the majority of the efforts have been focusing on an exposed region of this molecule, which mutates annually and frequently nullifies the existing flu inhibitors. The stem domain of HA (HA2), on the other hand, is evolutionarily conserved and can be served as the target for cross-protective antibodies. HA2 functions through a dramatic structural transition. Fundamentally, except for some piecemeal data, a coherent understanding of the physical mechanism underlying this transition and how that connects to viral invasion is still lacking. A complete knowledge of this could assist scientists in finding a long-lasting universal vaccine that can be effective towards various strains of flu viruses. Here we use computational tools of molecular dynamics to study the functionalities of HA2. Our simulations reveal a dynamical picture of HA2, which is causally related to the delivery of viral genomes. Our computations have also provided some metastable intermediates during the HA2 transition that can potentially serve as drug targets.

4D Compressive Imaging for Hyperspectral Video

Liyang Lu and Kevin F. Kelly

ECE Department, Rice University, Houston, TX, USA

Hyperspectral video imaging remains a challenging task given the high dimensionality of the datasets. Yet, it has great potential in studying dynamic optical phenomena with complicated spectral information, both in microscopic and macroscopic systems. Combining a new compressive imaging algorithm that is able to exploit the inherent redundancy in the temporal-spatio-spectral datacube with a unique optical system based on a single light modulator and a single detector, we are able to demonstrate a hyperspectral video imaging camera that compresses nearly 1000 to 1. With this system, it is possible to image molecular fluorescence and plasmon resonances in a dynamic environment from the ultraviolet to the mid-infrared spectrum.

Antioxidant Nanocarbon Therapy of Oxidative Stress in Mild Traumatic Brain Injury

Kimberly Mendoza,^{1,2} Leela Cherian Mathew,² Lizanne Nilewski,¹ William K. Sikkema,¹
Thomas A. Kent,² James M. Tour,¹

¹*Department of Chemistry, Rice University, Houston, TX, USA*

²*Department of Neurology, Baylor College of Medicine, Houston, TX, USA*

Hypotension worsens traumatic brain injury (TBI) and reactive oxygen species (ROS) contribute to loss of autoregulation and poor reperfusion. However, antioxidant therapy has not demonstrated clinical benefit. Most available antioxidants have limited capacity, narrow therapeutic range or require regeneration. We developed a novel carbon nanoparticle (PEG-HCCs) that is a catalytic antioxidant with broad and high capacity ROS-quenching. PEG-HCCs restored cerebral perfusion and improved functional outcome in mild TBI transformed to severe by hypotension/resuscitation. We hypothesized that the structural features we believe responsible for this remarkable efficacy could be mimicked in simpler materials more likely to achieve regulatory approval.

Graphitic quantum dots were prepared from bituminous coal under fuming nitric acid and compared to graphene-rich pegylated-Perylene diimide (PEG-PDI). 32 Long Evans rats underwent mild cortical compression injury. Regional cerebral perfusion was measured using Perimed laser speckle. In-vitro results in cultured neurons and brain endothelial cells indicated equivalent PEG-GQD potency to PEG-HCCs protecting against oxidative injury and both demonstrated catalytic superoxide-quenching activity. GQDs and PDIs were effective in restoring perfusion. Lesion size and neurological outcome measurements will be presented. Given that perfusion reduction is a major factor in worsening outcome after TBI, these agents deserve consideration as potential clinical therapeutics.

Tailoring development and processing of conjugated polymer binders for use in Si-based Li-ion battery anodes

Andrea Miranda,¹ Tracy Li,² Hyosung An,³ Jodie Lutkenhaus,³ and Rafael Verduzco²

¹*Department of Chemistry, Rice University, Houston, TX, USA*

²*Department of Chemical & Biomolecular Engineering, Rice University, Houston, TX, USA*

³*Department of Chemical Engineering, Texas A&M University, College Station, TX, USA*

Li-ion batteries are used in countless portable electronics and are making their way to larger-scale technologies like electric vehicles. To keep up with demand for a higher energy density battery, novel materials are being researched to optimize Li-ion battery performance. However, one often neglected component of Li-ion batteries, the polymer binder used in the electrodes, may hold the key to improved performance. Traditionally the role of the polymer binder has been limited to holding together the two other components of an electrode, the active material and conductive additive. But, if beneficial electrical and mechanical properties can be combined into a multi-functional polymer binder, it is possible that the amount of conductive additive can be reduced or removed altogether, increasing the overall energy density of the electrode. In this work, we synthesize a series of conjugated polymer-based binder materials for silicon anodes and also explore new ways to process commercially available conjugated polymers as binders. We cast electrodes through flow coating and compare their morphology, performance, mechanical properties, and electrochemical properties to state-of-the-art electrodes in the literature. Our work to date shows that the conductivity of the binder and battery performance is strongly dependent on doping and processing history, and the binder and electrode conductivity can be tuned over a wide range through variation of processing conditions. Current work is focused on systematic studies of battery performance with varying binder conductivity and investigation of electrode mechanical properties.

A Portable, Lower-Cost High-Resolution Microendoscope (PiHRME) to Screen for Cervical Cancer in Underserved Areas

Sonia Parra,¹ Pelham Keahey,¹ Kathleen Schmeler,² Mauricio Maza,³ Phil Castle,⁴ and Rebecca Richards-Kortum¹

¹*Department of Bioengineering, Rice University, Houston, TX, USA*

²*Department of Gynecologic Oncology & Reproductive Medicine, MD Anderson, Houston, TX, USA*

³*Basic Health International, San Salvador, El Salvador*

⁴*Department of Epidemiology & Population Health, Albert Einstein College of Medicine, Bronx, NY, USA*

There is a disproportionate incidence and mortality associated with cervical cancer with nearly 90% of cervical cancer deaths occurring in developing countries. Furthermore, there is evidence to show that there is a higher incidence of cervical cancer in rural areas of the United States such as the US-Mexico border. Even though the early detection and treatment of precancerous lesions can prevent cervical cancer, limited resources make it difficult to implement standard screening methods, such as Pap smears, in many underserved areas. The standard of care in many low-resource settings is a simple visual inspection of the cervix with acetic acid, however, this has the tendency to result in false cancer diagnoses and lead to the

overtreatment of women. We therefore have developed a low-cost, high-resolution microscope based on a single-board computer (PiHRME) to improve the sensitivity and specificity of detecting cervical precancerous lesions at the point-of-care. This device builds off past HRME models by making the HRME more affordable while maintaining high quality imaging for screening. This includes adapting and improving our automatic image analysis software to allow the PiHRME to better detect high-grade cervical precancerous lesions. By using the PiHRME, health care workers with minimal training will be able to image the cervix and analyze the images in real time to provide women with access to high-resolution cervical cancer imaging and screening at the point-of-care.

Design, Fabrication, and Characterization of 3D Printed Microscale Bicuspid Valves

Samantha Paulsen,¹ Bagrat Grigoryan,¹ and Jordan Miller¹

¹*Bioengineering, Rice University, Houston, TX, USA*

Bicuspid valves are essential structures within veins and lymphatic vessels, ensuring unidirectional flow of fluids back towards the heart. The failure of venous valves can result in chronic venous insufficiency (CVI), a disease which affects 2.5 million people within the United States, with symptoms ranging from varicose vein formation and edema, to ulceration, and chronic wound formation. Investigation of valve structure-function relationships is key for improving clinical treatments towards CVI; however, analyzing this structure function relationship of venous and lymphatic valves *in vivo* is hampered by the deep position of veins and lymphatics along with the dynamic nature of valves actuating above 1 Hz. Here, we sought to develop comprehensive *in silico* and *in vitro* models of microscale bicuspid valves to probe the relationship between valve architecture and fluid dynamics under pulsatile flow. We implemented computational fluid-structure interactions (FSI) models along with a 3D printing approach based on stereolithography to investigate microscale bicuspid valves.

This work demonstrates the feasibility of constructing computational FSI models to investigate structure function relationships in microscale bicuspid valves along with the fabrication of valve structures from biocompatible hydrogels using our new stereolithography-based 3D printing system.

Dynamics of stress response in *Mycobacterium tuberculosis*

Satyajit Rao,¹ Oleg Igoshin¹

¹*Department of Bioengineering, Rice University, Houston, Texas, USA*

To successfully colonize host bacterial pathogens must sense and adapt to several stress conditions such as damage to their cell membrane. In human pathogen *Mycobacterium tuberculosis*, disease causing agent of TB, response to membrane stress is coordinated by the gene regulatory network involving MprA/B two-component system and alternative sigma factor σ^E . Even though architecture of the underlying network is known, the roles of different layers of regulatory complexity such as transcriptional feedback and post-translational regulation are not

well understood. Using data on transcription time-course of *sigE* and *mprA* genes in response to membrane stress treatment we aim to uncover how network architecture shapes the observed response. We show that the two-component system functions in the parameter regime where its output (concentration of the phosphorylated MprA) is independent of its transcriptional levels. Such a regime is made possible by the bifunctionality of MprB as it also dephosphorylates phosphorylated MprA. We also demonstrate that phosphatase activity of MprB is essential for rapidly restoring pre-stress levels of transcripts following stress removal. Furthermore, bifunctionality eliminates possibility of bistability or hysteresis in the system, and facilitates a rapid response to stress. We report that increased cooperativity provided by σ^E regulation by its anti-sigma factor RseA improves fold induction of σ^E -induced genes. Lastly, positive feedback, though does not affect phosphorylated response regulator, increases dynamic range of activity under stress and eliminates delays in response. We conclude that features of stress response network such as positive transcriptional feedback, bifunctional activity of MprB and post-translational regulation of σ^E enable a fast, high fold-change response in stress-protective genes.

Accelerating gold nanorod seedless synthesis with nanomolar concentrations of poly(vinylpyrrolidone)

Katherinne Requejo¹, Anton Liopo¹, and Eugene Zubarev^{1,2}

¹*Department of Chemistry, Rice University, Houston, Texas, USA*

²*Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA*

A novel protocol has been developed for the seedless synthesis of gold nanorods (AuNRs) with hydroquinone (HQ) by using poly(vinylpyrrolidone) (PVP, 10 kDa) as additive. The polymer is introduced to growth solutions during synthesis of AuNRs for different concentrations of surfactant cetyltrimethylammonium bromide (CTAB): 25, 50 or 100 mM. Through the use of distinct CTAB and HQ concentrations, the LSPR band of AuNRs can be tuned from 700 to 1000 nm that corresponds to aspect ratio (length/width) from 2.61 ± 0.37 to 6.77 ± 0.73 . Kinetics experiments show that PVP accelerates the growth rate of AuNRs by more than two times for gold nanorods synthesized in 100 mM CTAB. By adding PVP, the original aspect ratio is reduced at different extents for each surfactant concentration. Thus, the synthesis produces AuNRs with dimensions from 17 x 4.8 nm to 43 x 7 nm for 50 and 100 mM and 12 x 4.5 nm for 25 mM CTAB. Moreover, the quality of AuNRs obtained in the presence of PVP is increased as compared to the control samples. The estimation of the average number of PVP chains per nanorod in solution indicates that around 10 to 50 molecules may interact with AuNRs and contribute to their stabilization. Because the concentration of PVP is far below the concentration of gold ions, 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.

Variance Spectroscopy: A New Bridge between Ensemble and Single-Particle Studies

Stephen R. Sanchez,¹ Jason K. Streit,¹ Sergei M. Bachilo,¹ and R. B. Weisman^{1,2}

¹*Department of Chemistry and the Smalley-Curl Institute, Rice University, Houston, TX*

²*Department of Materials Science and NanoEngineering, Rice University, Houston, TX*

Here we describe a new experimental technique, variance spectroscopy, which monitors many small regions of a bulk sample to extract spectral differences reflecting statistical variations in composition. The method is useful with samples, such as single-walled carbon nanotubes (SWCNTs), that show a distribution of spectral features arising from a distribution of nanoparticle structures. We quickly measure several thousand statistically independent emission spectra from different sample regions using custom instrumentation. The data are then analyzed to calculate the mean (first moment) and variance (second moment) of the emission intensity at each wavelength. Abundances of different SWCNT structural species and their relative emission efficiencies can be directly extracted from these mean and variance spectra. In addition, correlations between intensity fluctuations at different wavelengths provide further information, revealing the earliest stages of nanoparticle aggregation and giving spectra of homogeneous sub-populations within a well-dispersed sample. We have now applied variance spectroscopy in several SWCNT studies to determine absolute absorption cross sections for eleven different structural species, to measure salt-induced aggregation kinetics, and to study the effects of ultrasonication. Variance spectroscopy should become a practical and powerful experimental tool that can provide insights unavailable from bulk spectroscopy. A brief introduction to the method and its applications will be presented.

Aluminum Nanocrystals Decorated with Transition Metal Nanoislands as Antenna-Reactor Nanoparticles for Photocatalysis

Dayne F. Swearer,¹ Emilie Ringe,^{1,2} and Naomi J. Halas^{1,2,3}

¹*Department of Chemistry, Rice University, Houston, Texas, U.S.A.*

²*Department Material Science and Nanoengineering, Rice University, Houston, Texas, U.S.A.*

³*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, U.S.A.*

The ability to produce chemical fuels using a cheap, ubiquitous, and renewable energy source, such as the sun, has driven a worldwide search for new materials to secure a sustainable future. Our latest research efforts have focused on decorating Al nanocrystals with various transition metal islands (Pd, Pt, Rh, Ir, Ru, Fe, etc.) using a highly generalizable and adaptable polyol synthesis. In these heterometallic antenna-reactor nanoparticles, the Al nanocrystals act as an earth-abundant plasmonic antenna capable of harvesting energy directly from light, while the transition metals play the role of a highly reactive site for catalytic activity. The generalized nanoparticle synthesis method and results from morphological and compositional characterization using advanced electron microscopy will be presented. Then, mechanistic insights into the photocatalytic hydrogen-deuterium exchange and acetylene hydrogenation reactions on Al-Pd nanoparticles will be discussed, in addition to other potential reaction targets on Al-Ru, Al-Rh, and Al-Ni antenna-reactor nanoparticles.

Using imaging derived features to predict radiation response

Tien T. Tang¹, Janice A. Zawaski², Kathleen N. Francis¹, Amina A. Qutub¹,
M. Waleed Gaber^{1,2}

¹*Bioengineering, Rice University, Houston, TX, US*

²*Pediatrics, Baylor College of Medicine, Houston, TX, US*

Purpose: Medulloblastomas are the most common malignant central nervous system tumors in the pediatric population with radiotherapy being one of the main forms of treatment. These tumors are generally responsive to treatment but in some cases radioresistance or relapse can occur. However, current attempts at predicting treatment outcome relies on biopsies which has limited spatial and temporal resolution. MRI scans are commonly used and readily available in the clinic. In addition to anatomical information, MRI scans can be mined for features that are indicative of the underlying molecular activity and be used as predictive imaging biomarkers of treatment response.

Methods: Radioresistant cell line: Medulloblastoma cell line was treated with 2 Gy fraction irradiation and resistance was verified using a clonogenic assay. RT response model: mice were implanted in the cerebellum with Daoy cells suspended in matrigel. Animals received different RT protocols at 4 weeks post implant. T₁ weighted images with contrast was acquired before treatment and at approximately 1 week post treatment. The scans were mined for 26 imaging features, intensity and texture based, that were used to construct a decision tree for treatment outcome prediction.

Conclusion: Treatment response is dependent on time of treatment. Imaging features derived from texture analysis can capture distinct imaging signature between different treatment models. The decision tree is able to predict treatment outcome with 85% accuracy and with few imaging features. Future work will include identify imaging features of radioresistance and mining these features to develop a clinically relevant predictive model of radioresistance.

Pyrolytic Treatment of Soils Remediate Heavy Hydrocarbons and Enhances Fertility

Julia Vidonish¹, Kyriacos Zygourakis², Caroline A. Masiello³, and Pedro J.J. Alvarez¹

¹*Department of Civil and Environmental Engineering, Rice University, Houston, TX, USA*

²*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*

³*Department of Earth Sciences, Rice University, Houston, TX, USA*

Pyrolysis of biomass to produce biochar offers potential to improve soil agricultural quality and sequester carbon. Our research has integrated techniques frequently used in biochar production and soil remediation by thermal desorption to quickly remediate soils contaminated with recalcitrant heavy hydrocarbons from weathered oil spills. This approach preserves a fraction of soil organic carbon that are lost in other thermal technologies such as incineration.

We built a 0.5L fixed bed reactor to conduct bench-scale pyrolysis experiments, and determined appropriate processing conditions via thermogravimetric analysis. Plant toxicity studies were conducted using treated and untreated soils. Elemental analysis and SEM/FTIR microscopy are among the methods used to characterize pyrolyzed soils. Results show that pyrolysis is an

effective way to reduce TPH below regulatory levels without significant formation of PAHs. In addition, plant trials have shown higher biomass production in pyrolyzed soils over contaminated and incinerated soils. Characterization experiments are ongoing to describe the effect that pyrolysis has on remaining heavy hydrocarbons, soil density and mobility, and agricultural properties such as carbon content, water holding capacity, and cation exchange capacity. Results suggest that pyrolysis may have an important niche as a remediation strategy to quickly remove TPH below regulatory standards while preserving soil fertility and sequestering carbon.

Study of natural killer cell migration after tumor desensitization by shed NKG2D

Timothy Vu,^{1,2} Yuan Ma,² Ricardo Bessa de Castro,² and Lidong Qin²

¹*Department of Bioengineering, Rice University, Houston, TX, USA*

²*Department of Nanomedicine, Houston Methodist Research Institute, Houston, TX, USA*

Natural killer(NK) cells are a type of immune lymphocyte that plays a crucial role in the innate immune system and tumor defense. Recently, they have been studied as a possible cancer immunotherapy target and have undergone several clinical trials. One problem limiting treatment efficacy is tumor cells' ability to desensitize NK cells by releasing the ligands that regulate cytotoxicity, specifically ligands for NKG2D. This desensitization decreases NK cells' cytotoxicity and ability to maintain homeostasis. An area that hasn't been studied, however, is how this desensitization affects NK cells' potential to migrate and infiltrate tumors. The migratory and infiltration ability might explain NK cells' inability to fight solid tumors as efficiency *in vivo*. In this study, we demonstrate that shed MICA, a ligand to NKG2D, decreases NK cells' migratory ability significantly at clinically relevant concentrations. We then examine how using clinical cytokines for NK activation and enhancement, such as IL-2, IL-12, IL-15, and IL-18, affects NK cells' migration potential after MICA exposure, and how NK cells can influence cancer cells' shedding of NKG2D. Lastly, we will discuss our efforts in studying NK cell infiltration into cancer cells and our development of a 3D microfluidic model to study lymphocyte infiltration into solid tumor tissue.

Brain Modularity Mediates the Relation between Task Complexity and Performance

Fengdan Ye^{b,d}, Qiuhai Yue^a, Randi Martin^a, Simon Fischer-Baum^a, Aurora I. Ramos-Nuñez^a, and Michael W. Deem^{b,c,d}

^a*Department of Psychology, Rice University*

^b*Department of Physics & Astronomy, Rice University*

^c*Department of Bioengineering, Rice University*

^d*Department of Bioengineering, Rice University*

Recent work in cognitive neuroscience has focused on analyzing the brain as a network, rather than as a collection of independent regions. Prior studies taking this approach have found that individual differences in the degree of modularity of the brain network relate to performance on cognitive tasks. However, inconsistent results concerning the direction of this relationship have been obtained, with some tasks showing better performance as modularity increases and

other tasks showing worse performance. A recent theoretical model (Chen & Deem, 2015) suggests that these inconsistencies may be explained on the grounds that high-modularity networks favor performance on simple tasks whereas low-modularity networks favor performance on more complex tasks. The current study tests these predictions by relating modularity from resting-state fMRI to performance on a set of simple and complex behavioral tasks. Complex and simple tasks were defined on the basis of whether they did or did not draw on executive attention. Consistent with predictions, we found a negative correlation between individuals' modularity and their performance on a composite measure combining scores from the complex tasks but a positive correlation with performance on a composite measure combining scores from the simple tasks. These results and theory presented here provide a framework for linking measures of whole brain organization from network neuroscience to cognitive processing.

Quenching of Single-Walled Carbon Nanotube Fluorescence by Physisorbed Oxygen Reveals Selective ssDNA Affinities

Yu Zheng,¹ Sergei M. Bachilo,¹ and R. Bruce Weisman^{1,2}

¹*Department of Chemistry and the Smalley-Curl Institute and* ²*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, 77025*

Surface coatings on single-walled carbon nanotubes (SWCNTs) play key roles in their properties and applications. One of the most intriguing coatings is single-stranded DNA (ssDNA), which is known to helically wrap individual nanotubes with affinities that depend on oligonucleotide sequence and SWCNT structure. Based on the specific affinity, different nanotube species can be sorted by using specific ssDNA oligos through aqueous two-phase or chromatographic separation methods. However, identifying the selective affinity ssDNA sequences from an extremely large number of possible oligomeric compositions is time and money consuming. Here we report a fast, reliable, and nondestructive way to test the wrapping affinity for ssDNA on SWCNTs. We have discovered that fluorescence of ssDNA-wrapped SWCNTs is partially quenched by physisorbed O₂, and the extent of quenching measures affinities between ssDNA oligos and specific (*n,m*) SWCNT structures. We have investigated 10 different ssDNA sequences, and found the following specific recognition sequences: (ATT)₄ for (7,5), TTA(TAT)₂ATT for (6,5), and (TCG)₄TC for (8,6). We will present experimental results and a proposed mechanistic interpretation.