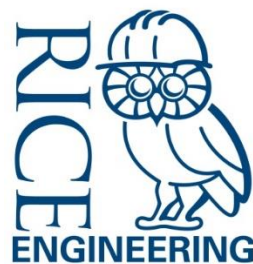# Colloquium III, August 11, 2017

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Event Catered by:

Presentation Schedule

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Oral Session 1A (Mabee Room 1070)

Session Chair: Charlotte Flatebo

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O-1A.1 - Optically controlled electrical switching by moving atoms: a multiscale modeling approach

A. Alabastri,[1] A. Emboras,[2] F. Ducry,[3] B. Cheng,[2] Y. Salamin,[2] P. Ma,[2] S. Andermatt,[3] C. Hafner,[2] M. Luisier,[3] J. Leuthold,[2] P. Nordlander[1]

[1]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[2] *Institute of Electromagnetic Fields (IEF), ETH, Zurich, Switzerland*
[3] *Computational Nanoelectronics Group, ETH, Zurich, Switzerland*

Shrinking devices dimension is one of the most important topics in the photonics and electronics industry. Smaller electrical and optical systems translate in energy savings and in larger densities of components that can be assembled together. Processors employing the latest 10-nanometer chip-manufacturing technology will probably start shipping during 2017. Every transistor update step leads chip makers closer to the fundamental limits where manipulation at the atomic level starts to emerge.

In this context, employing a platform which combines photonics and electronics at the atomic scale, we show how it is possible to optically induce an electronic switch by relocating one/few atoms. The device features a Si optical waveguide which carries an electromagnetic (EM) signal at 1.55μm. The EM signal is then squeezed, by means of an Ag covered tapered region, in a 20 nm thick and 100 nm wide SiO_2 layer which separates two metallic electrodes where a thin cone-shaped Ag filament was previously electrically formed. The light-to-heat conversion within the filament region induces the thin conductive element to dissolve, thus increasing by orders of magnitude the electrical resistance between the electrodes. Upon reduction of the input EM signal amplitude, the filament is re-built and the initial resistance conditions are restored. The filament rupture and reconstruction processes can be explained by the interplay of thermal diffusion, electrical forces and optical forces.

In particular here we show how a multiscale and classical modeling approach is capable to replicate the entire switching dynamics on a relatively long time scale of tens of seconds.

O-1A.2 - Light-Induced Band Gap Openings in Graphene

Bryan Anthonio,[1] Weilu Gao,[1] and Junichiro Kono[1,2,3]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[2]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[3]*Department of Materials Science and Nanoengineering, Rice University, Houston, TX, USA*

Graphene has recently emerged as one of the most studied materials in condensed matter physics due to its extraordinary electrical and mechanical properties that may be useful for many technological innovations. However, the fact that it lacks a bandgap renders it unfeasible for certain applications including optoelectronics and other semiconducting technologies such as fast-switching transistors.

Recent theoretical calculations have elucidated the possibility of opening a sizable bandgap by irradiating graphene with intense pulses of circularly polarized mid-infrared or far-infrared radiation through a coherent modification of the topological properties of electronic states. These studies predict that the size of the induced bandgaps varies with the wavelength and intensity of light excitations, which can be utilized to develop tunable and switchable optoelectronic devices. In this talk, we will describe our current efforts to experimentally demonstrate laser-induced bandgaps in graphene.

O-1A.3 - Assessing the effects of adsorption site clustering for chromatographic

separations

Logan D.C. Bishop,[1] Nicholas A. Moringo,[1] Hao Shen,[1]and Christy F. Landes[2]

[1]*Department of Chemistry, William Marsh Rice University, Houston, TX, USA*

Chromatographic separations represent a several billion-dollar expense in the pharmaceutical industry. While it has proven to be suitable for splitting a simple mixture into its constituent components it often lacks separation resolution in more complex systems. Overlapping of elution profiles, called tailing, reflects this loss of separability of the mixture components. Formation of elution profile tails is attributed to the presence of infrequent adsorption events that extend the elution time of a small subset of the eluent population. Single molecule studies have been employed as an empirical methodology for studying these events under the assumption that there are a variety of different adsorption sites with distinct adsorption/desorption times. Though this heterogeneity is reflective of the nature of the stationary phase, the possibility of longer binding times because of non-uniform site distribution has not been fully investigated. We assess the origins of tailing in a single site system where the local density of sites is the source of elongated elution times. This hypothesis is tested by Monte Carlo simulations of a single particle's 1D path through a chromatographic column where adsorption density of sites is variable along the trajectory. Organization of the stationary state is modeled by varying the placement of regions with many sites. Identifying the source of these elution effects, primarily if the heterogeneity of adsorption times is chemical or structural in nature, has applications in stationary phase engineering and eventually improvement in the overall separability of mixtures.

O-1A.4 - Evolution of Modularity for Frequency-Dependent Task Performance; Application to Understanding Cognitive Impairment in Alzheimer's

Melia E. Bonomo,[1,3] Michael W. Deem,[1,2,3]

[1] *Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*
[2] *Department of Bioengineering, Rice University, Houston, TX 77005, USA*
[3] *Center for Theoretical Biological Physics, Rice University, Houston, TX 77005, USA*

Alzheimer's disease (AD) is an increasingly prevalent condition worldwide characterized by progressive neural deterioration, and no definitive cause has been identified. Neuroimaging techniques that measure changes in neuron potentials, e.g., magnetoencephalogram (MEG), have revolutionized our ability to study brain activity at high temporal resolution. Brain regions that exhibit synchronized functional activity within a particular frequency band form a subnetwork. We analyze modularity as an informative network measure, the degree to which neural activity within a group of brain regions is more highly correlated than is activity between such groups. Interestingly, we analyze MEG data and find statistically significant higher modularity for AD patients compared to healthy controls in the low frequency bands and lower modularity for AD patients in the high frequency bands.

Previously we have theoretically derived and experimentally shown that healthy individuals with high whole-brain modularity perform better when completing tasks on shorter timescales, whereas on longer timescales, individuals with lower whole-brain modularity have higher performance. Here we adapt our theoretical model to consider how modularity varies within each frequency subnetwork of an individual to interpret the above mentioned MEG results for AD patients. I will present results from a model of evolving populations that shows modularity emerges on a frequency dependent spectrum, optimized for task performance, and effected by cognitive impairment.

O-1A.5 - A CMOS-Compatible Integrated IR Spectrometer

Benjamin Cerjan[1] and Naomi J. Halas[1,2,3,4]

[1]*Departmen of Physics and Astronomy, Rice University, Houston, TX, USA*
[2]*Department of Chemistry, Rice University, Houston, TX, USA*
[3]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[4]*Laboratory for Nanophotonics, Rice University, Houston, TX, USA*

We demonstrate an integrated room temperature infrared (IR) spectrometer, fabricated using complementary metal-oxide-semiconductor (CMOS) compatible processes. By using aluminum plasmonic gratings as combined filter elements and electrical contacts on a doped silicon substrate, we show that a low-cost IR spectrometer can be readily fabricated. As this spectrometer functions based on intra-band, or free carrier, absorption in silicon, it works well in to mid-IR "fingerprinting" region and has broad applications in chemical monitoring, e.g. environmental monitoring.

O-1A.6 - **Detection of antiferromagnetic order[1] and characterizing spin-charge separation[2] with ultracold ^{6}Li in a compensated optical lattice**

Ya-Ting Chang[1], Tsung-Lin Yang[1], Zhenghao Zhao [1], Chung-You Shih[1] and Randall G. Hulet[1]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, United States*

We explore the physics of fermions in both 1D and 3D using ^{6}Li atoms in an optical lattice. We have realized the 3D Fermi-Hubbard model and detected short-range antiferromagnetic (AFM) spin correlations via Bragg scattering[3]. We must cool the atoms to lower temperature to realize the long-range ordering. We are setting up a low noise laser and servo to reduce the rate of heating by the lattice intensity fluctuation.

In addition, we are also studying 1D system with two lattice beams. Luttinger liquid theory predicts that fermions have different speeds of sound for spin and charge excitations, an effect known as spin-charge separation. Evidence of spin-charge separation has been obtained in quantum wire tunneling experiments[4,5]. However, spin and charge dispersion have not been measured independently. Ultracold atoms provide a highly tunable system for which we may directly observe this phenomenon using Bragg spectroscopy[6].
Reference:

[1] Work supported by NSF and The Welch Foundation.
[2] Work supported by ARO MURI grant, NSF and The Welch Foundation.
[3] R. A. Hart, P. M. Duarte et al., Nature 519, 211-214 (2015).
[4]O. M. Auslaender et al., Science 308, 88 (2005).
[5] Y. Jompol et al., Science 325, 597 (2009).
[6] S. Hoinka et al., Phys. Rev. Lett. 109 , 050403 (2012)

O-1B.1 - **Determination of contrast factors for cubic slip-systems and their application in the microstructural characterization of binary Fm-3m materials**

Danyel Cavazos-Cavazos,[1] and Flavio F. Contreras Torres[2]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[2]*Centro del Agua para América Latina y el Caribe y Departamento de Física, Tecnológico de Monterrey, Monterrey, Nuevo León, Mexico*

Theoretical attempts to rationalize the strain anisotropy of crystalline systems in terms of dislocations often include the calculation of contrast factors. However, the evaluation of such parameters can be cumbersome because both elastic properties and symmetry restraints must be considered simultaneously, especially when calculating the distortion tensor and the elastic contributions in slip coordinate systems. In this study, a dislocation-dependent coordinate system is introduced to obtain straightforward expressions for the evaluation of individual contrast factors by a first principles approach. Herein, we report for the first time the contrast factors for KCl and NaCl regarding edge and screw dislocations; a further analysis of their microstructure was also carried out through the modified Williamson-Hall method.
https://doi.org/10.1016/j.jpcs.2017.05.027

O-1B.2 - **Towards quantitative Quantum Nanoplasmonics**

L. Bursi,[1] A. Calzolari,[2] S. Corni,[2,3] E. Molinari[2,4] and P. Nordlander[1]

[1]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[2]*CNR Institute of Nanoscience, Modena, Italy*
[3]*Department of Chemical Sciences, University of Padova, Padova, Italy*
[4]*Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia, Modena, Italy*

A recent trend in nanoplasmonics involves shrinking the size of plasmon-supporting nanostructures down to a few nanometers, thus enabling control over light-matter interaction at molecular scales.
On the theoretical side, the microscopic definition of plasmons in such molecular-sized nanostructures is a tremendous challenge.[1] Any sharp classification of the excitation nature (nonplasmonic vs plasmonic) becomes blurred in this limit, where quantum effects, such as nonlocal screening and size quantization, strongly affect the electronic excitation properties.
We recently introduced original microscopic approaches that ultimately provide a universal quantitative metric for the plasmonic character of optical excitations in ultrasmall nanostructures, providing physically sound tools to sort such excitations on the base of their "plasmonicity". This implied both the reformulation of existing concepts, such as the plasmonic electric field enhancement,[2] and the introduction of new descriptors, based on rigorous theoretical derivations, called plasmonicity indexes.[3]
Their application, starting from first-principles simulations based on (TD)DFT, allows us to quantify the plasmonic behaviour of metallic and semiconductor nanoclusters, prototypical C-based molecules, paradigmatic hybrid systems; and more generally of nanospheres described within the jellium model and larger nanoparticles characterized through classical electrodynamics, thus shedding new light on the nature of plasmonic excitations at the molecular scale.

[1] S. Bernadotte, *et al.*, *J.Phys.Chem.C* **117**,1863 (2013); E.B. Guidez, *et al.*, *Nanoscale* **6**,11512 (2014); E. Townsend, *et al.*, *J.Mater.Res.* **30**,2389 (2015).
[2] L. Bursi, *et al.*, *ACS Photonics* **1**,1049 (2014).

[3] L. Bursi, *et al.*, *ACS Photonics* **3**,520 (2016); R. Zhang, L. Bursi, P. Nordlander, *et al.*, *ACS Nano* 10.1021/acsnano.7b03421 (2017).

O-1B.3 - Lifetime Characterization of Molecular Plasmons

Kyle Chapkin,[1,5] Adam Lauchner,[1,5] Grant Stec,[2,5] Luca Borsi,[1,5] Yao Cui,[1,5] Peter Nordlander,[1,3,4,5] Naomi Halas[1,2,3,5]

[1]*ECE Department, Rice University, Houston, TX, United States*
[2]*Chemistry Department, Rice University, Houston, TX, United States*
[3]*Department of Physics and Astronomy, Rice University, Houston, TX, United States*
[4]*MSNE Department, Rice University, TX, United States*
[5]*Laboratory for Nanophotonics, Rice University, Houston, TX, United States*

Graphene has been shown to be an exceptional material for supporting plasmons, with a tunability ranging from the mid-infrared to terahertz frequencies by electrostatic or chemical doping. However, by limiting the scale of the system to only a few dozen carbon atoms it becomes possible to access visible resonances; this is the realm of polycyclic aromatic hydrocarbons (PAHs), which have many promising applications including electrochromics and photocatalysis. PAHs are commercially available in high purity, defect-free forms and can be regarded as molecular-scale, hydrogen-passivated graphene. Recent theoretical work has shown that molecular-scale systems are capable of supporting collective excitation modes indicative of plasmonic behavior, rather than just single electron transitions (SET). In particular, for PAHs, the addition/removal of even a single electron changes the electronic structure of the molecule such that low-energy collective excitations may arise. Following trends found in graphene on prolonged plasmon lifetimes, we have more directly probed the plasmonic nature of these systems by taking excited state lifetime measurements, via degenerate transient absorption spectroscopy, of three molecular plasmon systems: the anion states of anthanthrene, benzo[ghi]perylene, and perylene. Our studies into the ultrafast dynamics of these charged PAH systems has yielded exciting results and given further insight into their characterization. This investigation explores the ultrafast dynamics of the molecular plasmon system and illuminates the distinction of short-lived molecular plasmon excitations from long-lived single-electron excitation.

O-1B.4 - Chemical Decoration of Boron Nitride Nanotubes with Aliphatic Carbon Chains

Carlos A. de los Reyes,[1] Kendahl L. Walz-Mitra,[1] Ashleigh D. Smith,[1] Frank Frankovsky,[1] and Angel A. Martí[2]

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

Boron nitride nanotubes (BNNTs) present a unique set of properties such as high mechanical strength, high thermal conductivity and a uniform wide band gap. They also possess high thermal and chemical stability, property which also sets back a wide range of applications envisioned for this material. Due to their chemical inertness, functionalization has been challenging and scarce. Moreover, to the best of our knowledge, only one example on alkyl grafting has been published so far. Therefore, in this work, boron nitride nanotubes have been functionalized with dodecyl chains (f-BNNTs) using the Billups-Birch reaction, a very straight-forward method. The infrared spectrum of f-BNNTs show a new set of peaks in the 2820-3000 cm^{-1} region assigned to C-H stretching and evidence of sp^3 boron environment, aside from their typical vibrations. The TGA shows a 6.6% weight loss, indicating approximately 1 chain per 95 BN units. A new property of the modified material is its ability to disperse in more non-polar solvents, demonstrating that the alkyl chains help stabilize the tubes in such environments. Additional to these studies, by correlating microscopy with photoluminescence, we have found

how to tune the centrifugation force of dispersions to obtain individual tubes and hexagonal boron nitride-free material.

O-1B.5 - Symmetry Breaking and Restoration by Similarity Transformation

Matthias Degroote[1], Thomas Henderson[1,2], John Gomez[2], Matthew Hermes[1], Jacob Wahlen-Strothman[2], Ethan Qiu[1], Jinmo Zhao[1], Jorge Dukelsky[3], Gustavo Scuseria[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas*
[2]*Department of Physics and Astronomy, Rice University, Houston, Texas*
[3]*Instituto de Estructura de la Materia, CSIC, Madrid, Spain*

Symmetry conserving correlation methods perform well for weak correlation. In the strong correlation regime increasingly high levels of theory are needed to keep the same level of accuracy. This problem can seemingly be overcome by letting the reference state break symmetry. While giving accurate ground state energies at mean field cost, this sacrifices accuracy on most other properties in finite systems. Symmetry restoration can be performed by either increasing the level of theory or projection of the broken-symmetry ground state into a multi-determinant wave function. We have recently developed a method that expresses the symmetry projected wave function as a similarity transformation on the symmetry adapted reference state, which links traditional coupled cluster style correlation methods to symmetry projection. I will present the key concepts, examples of performance for different hamiltonians and the challenges we still face.

O-1B.6 – Developing a single particle description of the protein corona

Lauren Warning,[1] Q. Zhang, K. Kapoor, S. Chatterjee, R. Baiyasi, C. Landes, and Stephan Link[1]

[1]*Chemistry Department, Rice University, Houston, TX, USA*

Nanomedicine is a promising field, but interactions between nanoparticles (NPs) and the human body are not yet entirely understood. Heightened understanding of interactions like NP-protein (NPP) corona formation—in which blood serum proteins bind to NP surfaces—could lead to improvements in cellular targeting and other nanomedical procedures. *Ex situ* methods frequently used to study the NPP corona are useful, but they often lack important *in situ* information about the system. In the current work, *in situ* ensemble techniques are employed to investigate interactions between gold nanorods (AuNRs) and the three most abundant blood serum proteins (serum albumin, fibrinogen, and immunoglobulin G). Specifically, effects of relative protein concentration and competitive binding in the NPP corona system are explored by altering protein concentration, composition, and order of exposure with protein mixtures. Additionally, the validity of using a three-protein mixture as a model for blood serum is tested by comparing measurements of both scenarios. Overall, we hope to create an *in situ* ensemble description of individual and competitive serum protein binding in the NPP corona and to critique our model protein system.

O-2A.1 – **Studying Protein Structure through Hydrogen Exchange and Conformational Sampling**

Didier Devaurs,[1] Dinler Antunes,[1] Jayvee Abella,[1] Mark Moll,[1] and Lydia Kavraki[1]

[1]*Department of Computer Science, Rice University, Houston, TX, USA*

A protein's function is known to be modulated by changes in its three-dimensional structure. Studying this structure-function relationship requires gathering information about the protein's conformational space, i.e., the space of all possible states of the protein. Some information can be obtained experimentally, using techniques such as X-ray crystallography. Various computational methods, such as molecular dynamics, are also used to obtain structural information. However, experimentally observing and computationally modeling large proteins remain critical challenges for structural biology. Our work addresses these challenges by combining experimental and computational techniques to overcome their respective shortcomings. At one end of the experimental spectrum, X-ray crystallography yields atomic-resolution models, but is limited by high cost and low applicability. At the other end of this spectrum, hydrogen-exchange monitoring is cheap and easier to implement, but cannot produce structural models because of its low resolution. One side of our approach consists of developing computational methods to complement such low-resolution experimental techniques. As these computational methods suffer from the curse of dimensionality when applied to large proteins, the other side of our approach consists of guiding them with experimental data. Our group leverages robotics-inspired techniques to model and analyze protein structure, by implementing coarse-grained conformational sampling methods to explore a protein's conformational space. We have developed a computational framework, named Structured Intuitive Move Selector (SIMS) integrating sampling-based path-planning algorithms with the well-established Rosetta library for protein modeling. Here, we present three outcomes of our coupled approach combining SIMS on the computational side and hydrogen-exchange on the experimental side.

O-2A.2 – **Quantifying Remote Heating from Propagating Surface Plasmon Polaritons**

Charlotte I. Evans, [1] Pavlo Zolotavin, [1] Alessandro Alabastri, [1] Jian Yang, [1] Peter Nordlander, [1,2,3] and Douglas Natelson[1,2,3]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, United States*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, United States*
[3]*Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, United States*

We report a method to electronically detect remote heating from the excitation of propagating surface plasmon polaritons (SPP). The coupling between SPP and a continuous wave laser beam is realized using lithographically defined gratings in the electrodes of gold thin film "bow tie" nanodevices. The propagating SPPs couple optical energy into the nanowire constriction. This coupling causes the nanowire constriction to heat, which is detectable through changes in the device conductance. This heating has contributions from both thermal diffusion of heat generated at the grating and heat generated locally at the constriction by plasmon dissipation. Through computational modeling, it is determined that the main contribution to the nanowire constriction is due to the propagation of SPPs. Coupling optical energy into the constriction via propagating SPPs in this geometry produces an inferred temperature rise of the constriction a factor of 60 smaller than would take place if optical energy were introduced via directly illuminating the constriction. Remotely exciting the constriction using the grating approach provides a path for remote excitation of nanoconstrictions using

SPPs for measurements that usually require direct laser illumination, such as surface-enhanced Raman spectroscopy.

O-2A.3 – **Direct Observation of Cross-Polarized Excitons in Aligned Single-Wall Carbon Nanotubes**

Fumiya Katsutani,[1] Weilu Gao,[1] Kazuhiro Yanagi,[2] and Junchiro Kono[1]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[2]*Department of Physics, Tokyo Metropolitan University, Hachiouji, Tokyo, Japan*

Semiconducting single-wall carbon nanotubes (SWCNTs) possess rich optical properties arising from one-dimensional excitons with extremely large binding energies. Although much has been understood about the properties of excitons that are active for parallel-polarized light, excitons excited by perpendicular-polarized light have not been explored experimentally. Such "cross-polarized" excitons are predicted to exhibit strong many-body effects due to a combination of quantum confinement and Coulomb interactions. Here, we have directly observed cross-polarized excitons by investigating the polarization dependence of optical absorption in a film of highly aligned, single-chirality SWCNTs. As the angle between the polarization of the incident beam and the nanotube alignment direction was increased from 0 to 90°, a new peak (E_{12}) appeared and grew in intensity at the expense of the usual parallel-polarized excitons (E_{11} and E_{22}). The photon energy of the E_{12} peak was found to be between those of the E_{11} and E_{22} peaks. Together with the nematic order parameter of the aligned SWCNT film known from electron microscopy, these polarization-dependent absorption measurements allow us to determine the importance of the depolarizing dynamic screening effects on the electron-hole Coulomb interaction quantitatively. In addition, we will consider possible relaxation of selection rules due to tube-tube coupling in this densely packed SWCNT film.

O-2A.4 – **Understanding Catalyst Residue Inhibition of the Functionalization of Single Wall Carbon Nanotubes via Billups-Birch Reduction**

Varun Shenoy Gangoli,[1] Kevin Zhang,[2] David Pham,[2] Olawale Lawal,[3] Saunab Ghosh,[1] Robert H. Hauge,[1] W. Wade Adams,[3] and Andrew R. Barron[1,4]

[1]*Department of Chemistry, Rice University, Houston, Texas, USA*
[2]*Smalley-Curl NanoCarbon Center, Rice University, Houston, Texas, USA*
[3]*Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA*
[4]*Energy Safety Research Institute, Swansea University Bay Campus, Swansea, Wales, UK*

Note: Abstract withheld per request of presenter.

O-2A.5 – **Catalytic Role of Titanium in the Synthesis of Aluminum Nanocrystals**

Benjamin Clark,[1] Chris DeSantis,[2] Gang Wu,[3] Ah-Lim Tsai,[3] and Naomi Halas[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas, USA*
[2]*Dept. of Electrical & Computer Engineering, Rice University, Houston, Texas, USA*
[3]*Division of Hematology, Internal Medicine & Biochemistry and*
Molecular Biology Program, University of Texas Medical School, Houston, Texas, USA

Since Haber and Buhro's seminal work [1], the synthesis of aluminum nanoparticles by titanium(IV) isopropoxide catalyzed thermal decomposition of alane adducts has become the standard for high purity nanoscale

aluminum. Recently, monodisperse single crystal Al nanoparticles (nanocrystals) with controlled sizes have been synthesized by this approach for sustainable plasmonics, giving rise to applications including selective photocatalysis with antenna-reactor nanostructures [2-5]. To further tune and enhance the plasmonic response of Al nanocrystals, precise control of nanocrystal shape is desired. However, the underlying mechanisms for the synthesis of Al nanocrystals, particularly the catalytic role of the titanium(IV) isopropoxide, remain unknown. Here, we capitalize on reduction of Ti^{4+} compounds into d^1 Ti^{3+} species by complexation with AlL_3 (L = H, CH_3, ^iBu), to investigate the mechanism of Al nanocrystal synthesis using electron paramagnetic resonance spectroscopy. Preliminary results indicate for Ti^{3+}-AlH_3 complexes the unpaired electron is delocalized between Ti and Al atoms bridged by two hydrides. Reductive elimination of H_2 is hypothesized to produce low valent Al^+ compounds that rapidly nucleate into Al seeds, while simultaneously regenerating the Ti^{4+} species, completing the catalytic cycle of titanium in the synthesis of Al nanocrystals.

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Oral Session 2B: 10:45 am – 12:00 PM

O-2B.1 – Ultra-small Plasmonic Nanosensors for Cancer detection

Sangheon Han,[1,2] Stanislav Emelianov,[3] 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*
[3]*Electrical & Computer Engineering and Biomedical Engineering, Georgia Institute of Technology and Emory University School of Medicine, Atlanta, GA*

Surface plasmon resonance (SPR) is a non-radiative process that results in scattering and absorbance and highly appears in noble metallic nanoparticles such as gold. This leads to explore biomedical applications especially in diagnostic imaging. The efficacy of SPR is highly dependent on the size of the metallic nanoparticles. Big nanoparticles tend to create high SPR but are not clinically translatable due to accumulation of the body. On the other hand, the use of ultra-small nanoparticles (< 10 nm) can achieve favorable bodily excretion but may have very low SPR effect for detection. Here, I present molecularly targeted plasmonic nanosensors (MAPS) of two different sizes for sensitive detection of cancer cell in combination with darkfield (DF) and photoacoustic (PA) imaging. MAPS consists of either 5 or 40 nm gold nanoparticle cores conjugated with anti-epidermal growth factor receptor antibodies for molecular targeting of cancer cells; they are co-coated with PEG molecules for *in vivo* applications. DF imaging is commonly used in a laboratory bench to detect scattering portion of SPR from nanoparticles in a black background where the incident light is placed at an angle away from detection. PA imaging is a clinically translatable diagnostic imaging method that uses a near-infrared light to stimulate thermally tissues/cells or particles by absorption, which is detected as ultrasound.

The results show that 5 nm MAPS can generate comparable PA signals by absorption to 40 nm MAPS but not DF signals by scattering. In addition, PA imaging with 5 nm MAPS can allow detection of cancer cells with high sensitivity. 5 nm MAPS is likely to meet the threshold required for bodily excretion as well as highly sensitive cancer detection.

O-2B.2 – Spectral Response of Plasmonic Gold Nanoparticles to Capacitive Charging: Morphology Effects

Thomas Heiderscheit[1], Ben Hoener[1], Wei-Shun Chang[1], Stephan Link[1]

[1]*Department of Chemistry, Rice University, Houston, Texas*

Techniques used to study the catalytic activity of plasmonic nanomaterials on the single particle level typically utilize light through methods like dark-field scattering or fluorescence microscopy. These techniques lead to measured catalytic activity arising from both the molecule's affinity for certain facets of the nanoparticle crystal and the contributions from the plasmonic generation of hot carriers. One method for separately comparing the catalytic contributions of the molecules affinity for the surface and the generation of hot carriers is through electrogenerated chemiluminescence (ECL) microscopy. This method entails generating light through the redox reaction of $Ru(bpy)_3^{2+}$ with coreactant tripropylamine. Measuring the generated ECL intensity with and without laser excitation will allow for the comparison of catalytic activity arising from the molecular affinity and hot carrier generation respectively. The work presented shows experimental optimization of ECL conditions without light excitation and preliminary data with light excitation.

O-2B.3 – Synthesis and Optoelectronic Properties for P3HT Based Conjugated Block Copolymer with Flexible Linking Groups

Zhiqi Hu,[1] Jacek Jakowskij,[2] Bobby G. Sumpter,[2] Chenyu Zheng,[3] Christopher J. Collison,[3] Joseph W. Strzalka,[4] and Rafael Verduzco[1]

[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[2]*Computer Science and Mathematics Division, Oak Ridge Natinal Laboratory, Oak Ridge, TN, USA*
[3]*School of Chemistry and Materials Sciences, Rochester Institute of Technology, Rochester, NY, USA*
[4]*Division of X-ray Science, Argonne National Laboratory, Lemont, IL, USA*

State-of-the-art organic photovoltaics (OPVs) are prepared by depositing a disordered, co-continuous donor and acceptor blend. While optimization of material processing has produced significant improvements in performance, a fundamental understanding of charge separation and recombination at the donor/acceptor interface is lacking. Block copolymers with donor and acceptor polymer blocks provide an opportunity for controlling the donor-accepter interfacial structure and understanding its relationship to charge separation and photovoltaic performance. Here, we report the synthesis and characterization of donor-*linker*-acceptor block copolymers for use in OPVs. A series of poly(3-hexylthiophene)-block-poly((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(thiophen-5-yl)-2,1,3-benzothiadiazole]-2′,2″-diyl) (P3HT-PEG-PFTBT) are synthesized with flexible oligo-ethylene glycol (PEG) linkers. Photoluminescence measurements and density functional simulations demonstrate that the insertion of a non-conjugated linker has an insulation impact on energy transfer between the two blocks. Same result can also be verified through device test using block copolymers as additives for bulk heterojunction OPVs. This work provides insight into the charge separation process and demonstrates a technique for tailoring the donor-accepter interface in OPVs.

O-2B.4 – Borophene polymorphs for visible range plasmonics – a first-principles exploration

Yuefei Huang,[1] Sharmila N. Shirodkar,[1] and Boris I. Yakobson[1]

[1]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA*

Recently discovered two-dimensional (2D) boron polymorphs, collectively tagged borophene, are all metallic with high free charge carrier concentration, pointing towards possibility of supporting plasmons. Ab-initio linear response computations of the dielectric function allow one to calculate the plasmon frequencies (ω) in the selected example-structures of boron layers. The results show that the electrons in these sheets indeed mimic a 2D electron gas, and their plasmon dispersion in the small wavevector (q) limit accurately follows the signature-dependence $\omega \propto \sqrt{q}$. The plasmon frequencies that are not damped by single particle excitations do reach to the near infrared and even visible regions, making borophene the first material with 2D plasmons at such high frequencies, notably with no necessity for doping. The existence of several phases-polymorphs, with varying degree of metallicity and anisotropy, can further permit to fine tune plasmon behaviors in borophene—potentially a tantalizing material utility in nanophotonics.

O-2B.5 – Biomimetic, Strong, Tough and Self-healing Materials from Universal Sealant-Loaded, Porous Building Blocks

Sung Hoon Hwang[1], Joseph B. Miller[2] and Rouzbeh Shahsavari[1,2]
[1]*Materials Science & Nanoengineering, Rice University, Houston, Texas, United States*
[2]*Civil and Environmental Engineering, Rice University, Houston, Texas, Unites States*

Calcium-silicate based materials are applied in diverse industries due to their excellent strength, thermal stability and biodegradability. However, they are prone to various forms of mechanical damage due to inherent brittleness. Consequently, they would largely benefit from enhanced mechanical properties and also, self-healing capability. Herein, we present for the first time a unique bottom-up fabrication of biomimetic calcium-silicate composite, comprising uniformly-sized calcium-silicate porous nanoparticles (CPNPs) loaded with organic sealant. Similar to organic adhesives existing between nacre platelets in natural abalone shells, the organic sealant here serves as glue between the particles, directly leading to the enhanced micromechanical properties. Control over CPNP morphology, monodispersity and pore size is achieved through a refined solution-based synthesis, allowing 'direct impregnation' loading of sealants. The sealant-loaded nanoparticles are assembled under external pressure to generate a bioinspired structure, where the gluing effect of organic sealant induces 258% and 307% increase in indentation hardness and elastic modulus respectively compared to a reference sample produced without organic sealant. Furthermore, heating the damaged sample triggers further release of nanoconfined sealant to the surrounding areas and full curing therein. This results in 16.6% increase in compressive strength and 36.3% increase in toughness compared to a reference sample, confirming the complete structural and mechanical recovery. Overall, the positive results demonstrate a unique, bottom-up pathway towards developing a mechanically-enhanced calcium-silicate based material with self-healing capability to heat stimulus.

Keywords: Self-healing, biomimetic, calcium-silicate porous nanoparticles

Undergraduate (UG) Poster Session Abstracts

UG-01   **Phase Behavior of CNT Liquid Crystalline Solutions and Solution Processing into Capacitive Pressure Sensors**

Evan Biggers,[1] Vida Jamali,[1] Francesca Mirri,[1] and Matteo Pasquali[1,2]
[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX 77005*
[2]*Department of Chemistry, Rice University, Houston, TX 77005*

Carbon nanotubes (CNTs) are 100 times stronger than steel, as conductive as copper, and have a thermal conductivity 3 times that of diamond, all while being extremely lightweight. These spectacular properties make CNTs the perfect material for producing durable, flexible pressure sensors, which can be used in applications ranging from wearable electronics to human-like robotics. To translate the molecular properties of CNTs to the macro scale, it is important to use long, defect-free CNTs. By dissolving CNTs in chlorosulfonic acid, we are able to effectively process them into macro materials. We use extensional rheology and polarized light microscopy to determine CNT aspect ratio and solution morphology. Once characterized, the solution can be sheared to create highly aligned, flexible CNT films. By separating two films with an equally flexible dielectric material, we can create a durable, reversibly flexible capacitor that can be used as a pressure sensor.

UG-02   **A Convolutional Neural Network-based Algorithm for Targeting Relevant Diagnostic Sites in High-Resolution Microendoscope Images**

David Brenes,[1] Eric Yang,[2] Nadarajah Vigneswaran,[3] Ann M. Gillenwater,[4] and Rebecca Richards-Kortum[2]
[1]*Biomedical Engineering, Duke University, Durham, NC, USA*
[2]*Bioengineering, Rice University, Houston, TX, USA*
[3]*School of Dentistry, University of Texas, Houston, TX, USA*
[4]*Head and Neck Surgery, MD Anderson Cancer Center, Houston, TX, USA*

While treatable in early stages, oral cancer mortality rate remains high due to late diagnosis. The high-resolution microendoscope (HRME) is an optical diagnostic capable of imaging proflavine stained nuclei that are analyzed by automated algorithms for early diagnosis at the point-of-care. However, nuclei in these images are often obscured by debris and keratin, impeding accurate analysis. To address this issue, we developed a convolutional neural network (CNN)-based algorithm to identify regions within HRME images where nuclei are obscured and must not be analyzed.

HRME images are processed in three steps. First, the CNN processes overlapping sub-images and outputs a probability that nuclei are visible in the sub-image. Then, a probability map for the entire HRME image is generated. Finally, the probability map is thresholded to exclude nuclei obscured regions. The CNN was generated by fine-tuning a pre-trained AlexNet. Using the AUC performance metric, 5-fold cross validation was used to optimize the learning rate, select an epoch, and predict the generalization performance of the CNN. The heat map binarization threshold was set as the threshold generating the maximum balanced accuracy relative to the ground truth.

Epochs peaked at a validation AUC of 0.9568 when training at the optimized learning rate of 0.001. The average balanced accuracy across validations at the optimal thresholds was 0.90668. These metrics highlight the success of the CNN-based algorithm to identify regions of HRME images with obscured nuclei. This technique will allow existing automated algorithms to only process nuclei visible regions, thereby potentially deliver more accurate diagnoses.

UG-03   Patterning Vertically Aligned Single Walled Carbon Nanotubes

Savannah Cofer,[1,2] An Hua,[3] Clement Delacou,[3] Keigo Otsuka,[3] Rong Xiang,[3] and Shigeo Maruyama[3,4]

[1]*Department of Mechanical Engineering, Rice University, Houston, TX, USA*
[2]*Nakatani RIES: Research & International Experiences for Students Fellowship in Japan, Rice University, Houston, TX, USA*
[3]*Department of Mechanical Engineering, The University of Tokyo, Tokyo, Japan*
[4]*Energy NanoEngineering Laboratory, National Institute of Advanced Science and Technology (AIST), Tsukuba, Japan*

Single-walled carbon nanotubes (SWNTs) are considered one of the most promising materials for next generation optical and electronic devices, but their potential is currently limited by the gap between their high-performance nanoscale properties and their less impressive macroscale performance [1]. Previously, using water vapor treatment to form vertically aggregated SWNT walls on a buckypaper bottom in a micro-honeycomb network (μ-HN) has been successful in creating a material with lower sheet resistance and higher optical transmittance than buckypaper [2]. However, it is very difficult to control the size and uniformity of SWNT walls using only the evaporation and condensation of water as a building tool. In order to provide a template for this naturally occurring vertical aggregation, we investigated using micro-scale patterns created by photolithography to mechanically stamp forests of VA-SWNTs into the desired form, prior to water treatment. We found that these patterned materials exhibit greater transparency and lower sheet resistance than both unstamped and untreated VA-SWNTs, which is promising for applications as a transparent conductor and in Si-SWNT solar cells. Since parameters such as cell size and shape, force applied, and cell depth can be better controlled with patterning, perhaps technique is promising for further optimization of μ-HN morphology for a wide variety of applications.

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UG-04   Analyzing the Response of the Scintillation Attenuation Spectrometer for Short-Pulse Ultra-Intense Gamma-Ray Sources

Andriy Dashko,[2] Edison Liang,[1] Kelly Yao,[1] Yingchao Lu,[1] Aileen Zhang,[3] Gary Wong,[4] Allen Mao,[1] Omar Garcia,[1] Peter Buckman,[3] and Kevin Jung[3]

[1]*Department of Physics and Astronomy, Rice University, Houston, TX, U.S.A.*
[2]*Department of Electrical and Computer Engineering, University of Texas at Austin, Austin, TX, U.S.A.*
[3]*St. John's School, Houston, TX, U.S.A.*
[4]*Department of Cancer Systems Imaging, The University of Texas MD Anderson Cancer Center, Houston, TX, U.S.A.*

Many gamma ray detectors exist to obtain gamma-ray spectra from sources that individually count the photons emitted by scintillators, but the experiment at Texas Petawatt Laser (TPW) demanded a spectrometer that can detect the gamma-ray spectrum created by the short-pulse ultra-intense laser irradiating solid high-Z targets. The scintillation attenuation spectrometer (SAS) was created to solve this challenge because even under the TPW experiment conditions, it produces a usable response. The SAS consists of an array of 36 x 48 LYSO scintillator crystal pixels partitioned with reflective foils to isolate the optical photons in each pixel, which is coupled to a CCD camera. The gamma rays from the experiment are collimated to produce a 2D light pattern in the pixels that is recorded by the camera, and this light pattern response corresponds to the gamma-ray spectrum produced by the experiment. The goal of the analysis on the SAS is to accurately recreate the gamma-ray spectrum based on the produced light pattern. Our analysis made use of GEANT4, a Monte Carlo simulation code for high-energy physics, to simulate the detector's response to monoenergetic gamma ray sources to create

a detector response matrix (DRM). The DRM was then used on experimental and simulation signals from the SAS to reconstruct the gamma-ray spectrum using the techniques of unfolding and forward folding.

UG-05   ARPES Investigation of Pseudogap in Bi2212

William Funkenbusch[1,2], R. Sobota[3], and T. Takeuchi[3]
[1]*Chemical Engineering Department, University of Rochester, Rochester, NY, USA*
[2]*Nakatani Research and International Experience for Students Fellowship in Japan, Rice University, Houston, TX, USA*
[3]*Energy Materials Laboratory, Toyota Technological Institute, Toyota, Japan*

Cuprate superconductors are characterized by high critical temperatures exceeding liquid nitrogen temperature (77K), giving them a strong potential for industrial applications. However, a dip in the density of electronic states near the Fermi energy, named the pseudogap, was found to reduce the number of electrons contributing to the superconducting state, and, as a result, decrease the critical temperature. A better understanding of the pseudogap and superconducting states may allow the critical temperature of these superconductors to be further increased. The current study employed Angle-Resolved Photoemission Spectroscopy (ARPES) to characterize the superconducting gap and pseudogap of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212), a high critical temperature cuprate superconductor. A high-quality single crystal sample of optimally doped Bi2212 (Pb = 0.4, Y = 0.05) was prepared by the Traveling Solvent Floating Zone (TSFZ) technique. Its orientation and crystallinity were confirmed via X-Ray Diffraction (XRD). The sample's electron transport and thermodynamic properties (electrical resistivity, magnetic susceptibility, and Seebeck coefficient) were measured over a wide temperature range from 5 to 300 K. Finally, ARPES measurements were performed to investigate the energy-momentum dispersion of conduction electrons in close vicinity to the Fermi energy. These measurements allowed us to study the evolution of the pseudogap and superconducting gap as a function of temperature and Fermi vector on the 2D Fermi surface. Ultimately, it is hoped that this work will lead to a better understanding of cuprate superconductivity in the optimally doped regime.

UG-06   Observing and Modelling Synchronization Phenomena in Oscillatory Systems

Jakob Grzesik,[1,2] M. Shoufie Ukharty,[3] and Riichiro Saito[3]
[1]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, U.S.A*
[2]*Nakatani RIES: Research & International Experience for Students Fellowship in Japan, Rice University, Houston, Texas, U.S.A.*
[3]*Department of Physics, Tohoku University, Sendai, Miyagi, Japan*

Synchronization, a phenomenon in which two or more objects in a system act in unison, is prevalent throughout nature. Examples include an audience's applause, which synchronizes after a short period to create a single, large, regular rhythm of clapping[1]; the illumination provided by many fireflies[2], which may eventually begin emitting light in unison. Interest in the synchronization phenomenon in physics began with observations of pendulum synchronization on a ship by Dutch physicist Christiaan Huygens in the 17th century[3]. Synchronization is also prevalent in solid state physics, and is an important component of studies in plasmons[4], and the coherent phonon phenomenon[5] in a system of carbon nanotubes with synchronized radial breathing modes. In order to understand synchronization in these types of systems, we consider a model which consists of a group of oscillators interacting with each other through an oscillating substrate. Each oscillator is modelled by a mass m attached to a spring with a spring constant of k and a damping factor of γ. We expect that these parameters affect the synchronization. Using analytical mechanics, we determine the equations of motion for each of the small particles' positions as a function of time through numerical calculations by solving coupled differential equations using the Runge-Kutta approximation method, implemented through Python programming. Defining synchronization time to be the time it takes for a system of small oscillators to have the same displacement from equilibrium, we've found a link between k, m, and γ and the synchronization time.

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UG-07   Mitral valve co-culture model in 3-Dimensional hydrogels

Mina Hemmati, [1] Amadeus Zhu, [1] Jane Grande-Allen[1]
[1]*Bioengineering, Rice University, Houston, Texas, United States*

Mitral regurgitation is a disease that affects the normal function of the mitral valve by causing blood to leak backward. For severe mitral regurgitation, surgery to repair or replace the valve is often needed. Therefore, we would like to find new treatments using drugs instead of surgery. Three-dimensional hydrogels allow us to mimic the ECM and examine different drugs in order to find a suitable treatment.

We isolated primary cells from pig hearts. There are two types of cells in the heart valve: valvular endothelial cells (VECs) and valvular interstitial cells (VICs). VICs are the fibroblast-like cells that populate the interior of the heart valve, while VECs are endothelial cells that line both surfaces of the valve.

To prepare a model that mimics the structure of valves with these layers, we grew the cells on 3-dimensional (PEG) hydrogels. We used PEG because it allows us to attach different peptides to the scaffold.

Overall, we isolated cells, sorted cells using beads, counted cells, passaged cells, and prepared the hydrogel co-culture model. We successfully attached VICs to the interior of the gel. For the next step, we are doing this experiment in hydrogels of different stiffness. However, we did not successfully attach VECs on the surface of the hydrogel, because we had problems with the cell morphology. We tried to optimize the protocols in order to improve cell attachment. Eventually, we will include both VECs and VICs in our 3-dimensional co-culture, like they are in the valve.

UG-08   Terahertz Spectroscopy of High-Temperature Superconductor Yttrium Barium Copper Oxide in High Magnetic Fields up to 30 T

Jeffrey Horowitz,[1] G. Timothy Noe[1], and Junichiro Kono[1]
[1]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*

Although discovered 30 years ago, high-temperature superconductors are still a subject of ongoing research, with the physics not yet fully understood. More recently they have been studied for use in metamaterials and terahertz (THz) generation. With our setup for single-shot THz time-domain spectroscopy capable of performing optical-pump/THz-probe experiments in high magnetic fields, we measured the THz response of the high-temperature superconductor yttrium barium copper oxide (YBCO) in magnetic fields up to 30 T. In the setup, the output beam from a chirped pulse amplifier is split into two parts, one which is used to generate THz and another which is used to probe THz radiation. THz radiation is generated using a ZnTe crystal to achieve a bandwidth of ~2.5 THz. To increase the amplitude of the higher-frequency components of the THz generated, we designed a cryostat to lower the temperature of the ZnTe crystal. Once the THz radiation is generated, the THz passes through a sample placed in a magnet, and the results are imaged onto a camera. Using liquid nitrogen, we cooled the YBCO sample to about 77 K, which is below the critical temperature, therefore causing the sample to be superconducting. As a type-II superconductor, YBCO has two critical

magnetic fields between which the superconductor is in an intermediate state where some magnetic flux can pass through the sample. Because the second critical field of YBCO is below 30 T at 77 K, we tuned the magnetic field through all three states of the superconductor.

UG-09   **Design of Microwave Antenna for Orbital Angular Momentum Transfer Research Using Electron Spins in Diamond**

Rose Huang,[1,2,3] Kento Sasaki,[3] Eisuke Abe,[3] Yasuaki Monnai,[3] and Kohei M. Itoh[3]

[1]*Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York, U.S.A.*
[2]*Nakatani RIES: Research and International Experience for Students Fellowship in Japan, Rice University, Houston, Texas, U.S.A.*
[3]*School of Fundamental Science and Technology, Keio University, Yokohama, Japan*

Nitrogen vacancy (NV) defects in diamond have promising applications in quantum information processing and quantum sensing. Electrons of a NV center form a spin-1 system, and can be excited from $m_s = 0$ to $m_s = \pm 1$ using circularly polarized microwaves. We can readout the final spin state with photoluminescence (ODMR: optically detected magnetic resonance). The transfer of orbital angular momentum to spin angular momentum in a NV center will enable larger transitions between spin states. We report on a microwave antenna that generates a twisted magnetic field. The design consists of 8 copper loops on a square FR-4 substrate with a layer of copper behind it. There is a linear phase delay between each excitation port attached to the end of the copper loops. Simulated on CST MICROWAVE STUDIO®, this antenna emits 2 GHz twisted microwave with a 4π rotation. We expect that the antenna will excite electrons from $m_s = -1$ to $m_s = +1$ for a (111)-oriented diamond. The excitation of the NV center will be assessed with twisted microwave light by an ODMR setup. The electrons of the NV center will be excited from $m_s = 0$ to $m_s = -1$ with linearly polarized microwaves, and then further excited from $m_s = -1$ to $m_s = +1$ using the twisted light microwave antenna. This additional transition between the NV spin states will allow for increased sensitivity in NV-based sensors.

UG-10   **Exciton Linewidth Effects on Valley Relaxation in 2D TMDCs**

Alexander Hwang[1,2,3], Wenjin Zhang[4], Kazunari Matsuda[4], and Yuhei Miyauchi[4]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, U.S.A.*
[2]*Department of Physics, Rice University, Houston, TX, U.S.A.*
[3]*Nakatani RIES: Research and International Experience for Students Fellowship in Japan, Rice University, Houston, TX, U.S.A.*
[4]*Institute of Advanced Energy, Kyoto University, Kyoto, Japan*

Monolayer transition metal dichalcogenides (TMDCs) have shown exceptional promise as valleytronic materials. Their strongly coupled spin-valley physics allow selective valley population using circularly polarized light. Understanding the physical mechanisms behind valley relaxation (loss of binary valley information) in these materials is an important, ongoing research topic. We have accumulated experimental evidence for a comprehensive theory [1] of two-dimensional screened, electron-hole exchange-interaction-mediated valley relaxation processes in TMDCs [2]. Our results can also explain temperature-dependent and excitation-density-dependent valley relaxation phenomena in a variety of previous studies. According to our theory, valley relaxation times should show strong dependence on exciton homogeneous linewidth. Through changing excitation density with a pulsed laser, we recently showed an inverse relationship between steady-state valley polarization and exciton homogeneous linewidth at low temperature, consistent with our theory. We also showcase recent efforts to enhance valley physics by encapsulating TMDCs in thin layers of hexagonal boron nitride (hBN). This is a common practice for enhancing the optical and electronic properties of graphene,

but has been only recently been utilized for TMDCs. We demonstrate the effects of hBN encapsulation on improving low-temperature excitonic spectra of monolayer MoS_2, and report on how this affects valley relaxation physics within the context of our current theoretical understanding. Our results help gain insight into the fundamental valley physics of monolayer TMDCs, a class of exciting valleytronic materials.

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UG-11   Functional Architectures of Aligned Carbon Nanotubes

Natsumi Komatsu,[1] Weilu Gao,[1] Peiyu Chen, [1] Cheng Guo, [2] Aydin Babakhani, [1] and Junichiro Kono[1]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[2]*Department of Applied Physics, Stanford University, Stanford, CA, USA*

We have fabricated a novel structure consisting of multiple thin (≈ 20 nm) layers of aligned single-wall carbon nanotubes (SWCNTs) with dopants inserted between the layers. The individual carbon nanotube films—highly aligned, densely packed, and large (2 in. in diameter)—were produced using vacuum filtration [1] and then stacked together in the presence of dopants [2]. Dopants were incorporated into the structure in such a way that they reside between the conducting layers, effectively increasing the conductivity of the layers. This unique 3D architecture of doped SWCNTs exhibited excellent performance as a terahertz (THz) polarizer with an ultrabroadband working frequency range (from 0.2 to 200 THz), a high extinction ratio (20 dB from 0.2 to 1 THz), and a low insertion loss (<2.5 dB from 0.2 to 200 THz), exceeding the performance of previously reported THz polarizers using SWCNTs. Our basic fabrication procedure is general and can in principle be extended with no limitations in size and complexity to achieve more complicated and larger structures containing aligned SWCNTs. Furthermore, we have fabricated an aligned film of dye-inserted SWCNTs, in order to realize a giant polarization by taking advantage of recently reported ultrahigh hyperpolarizability of individual SWCNTs containing DANS molecules. We conducted oxygen plasma treatment to the filter membrane to change and optimize the surface potential for DANS-inserted SWCNTs and obtained a reduced linear dichroism of 0.57.

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UG-12   Fluorescence-enhanced silver on gold nanoclusters for optical sensing applications

Fernando Lejarza,[1] Christian L. Conrood,[1] Yinyuan "Ben" Yin[1], Michael S. Wong[*1,2,3,4]

[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, United States*
[2]*Department of Chemistry, Rice University, Houston, TX, United States*
[3]*Department of Civil and Environmental Engineering, Rice University, Houston, TX, United States*
[4]*Department of Materials Science and Nanoengineering, Rice University, Houston, TX, United States*

Gold nanoparticles (NPs) larger than ~2 nm have been utilized for electronics and microscopy due to their plasmonic nature - exhibiting a semi-continuous electronic structure. Atomically precise metal NPs with sizes less than ~2 nm, however, were found to contain discrete electronic states due to strong quantum confinement [1]. These noble metal nanoclusters (NCs) with core sizes < 2 nm display strong photoluminescence properties and hold incredible promise for optical sensor, bioimaging and catalysis applications [2] [3]. Unfortunately, their low quantum yield (QY) (~8%) has limited their implementation. To overcome this, thiol groups (SR-), such as glutathione (GHS), are used to cap NCs (SR-NCs) resulting in greater stability, enhanced QY (~15%) and new structural properties [4] [5]. Our early work utilized gold (Au)

NCs to detect the highly carcinogenic contaminant chromium(VI) (Cr(VI)) in water. In this work, the QY of the Au NCs has been substantially enhanced by depositing silver (Ag) atoms in the Au core: resulting in a 2-fold increase in fluorescence intensity and enhanced Cr(VI) sensitivity. It is estimated that the silver deposition on core of the original Au NCs ($Au_{29-43}(GHS)_{27-37}$) yields a bimetallic NC ($Au_{29-43}Ag_{3-38}(GHS)_{27-37}$). Not only does this work demonstrate a greatly improved sensor at the mere cost of one additional synthesis step, but the bimetallic core results in a peak emission shift from 610 nm (orange/yellow) to 622 nm (red). This observation indicates that bimetallic NC hold great promise for the design of sensors with tunable emission and optoelectronic properties.

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UG-13   Exploration of Charge Dynamics of Well-Aligned CNT (6,5) Through THz Generation

Aaron Ludvigsen,[1,2] Bagsican Filchito Renee G,[3] Weilu Gao,[4] Iwao Kawayama, [3] Junichoro Kono,[4] Masayoshi Tonouchi,[3] and Robert Vajtai[5]

[1]*Department of Physics, Bethel University, St Paul, MM, USA*
[2]*Nakatani RIES: Research and International Experience for Students Fellowship in Japan, Rice University, Houston, TX, USA*
[3]*Institute of Laser Engineering, Osaka University, Suita, Osaka, Japan*
[4]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[5]*Department of Materials Science & NanoEngineering, Rice University, Houston, TX, USA*

Homogenously aligned carbon nanotube (CNT) films are able to accentuate the unique anisotropic properties of individual CNT and allow for greater control of these qualities. Knowing these characteristics will help us understand more about the applications of homogenously aligned CNT films. This research will explore the charge dynamics of CNT. Using CNT in a photo-antenna, THz radiation was produced and detected through terahertz time-domain spectroscopy (THz-TDS). Variations included the polarization of the light falling on the sample, the alignment of the photoconductive antenna (PCA) with respect to the aligned CNT, and the voltage bias applied to the PCA. Further variation of the pump wavelength is expected to cause changes in the excitation and relaxation times of the CNT. This research allows for the exploration of the anisotropy of CNT, the efficiency of photon generation and generation of THz radiation, and the ease of breaking the electron-hole pairs in CNT.

UG-14   Micron-scale Structure in Carbon Nanotube Liquid Crystal Droplets

Miranda Mittleman[1] Vida Jamali[1] Vicki Colvin[2] and Matteo Pasquali[1]

[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston TX*
[2]*Department of Chemistry, Brown University, Providence RI*

Carbon nanotubes (CNT) are a type of nanomaterial with unique properties, which give them a potential to be useful in a variety of applications. Solution processing of CNTs is a versatile method to make CNT-based macromaterials including fibers, films, sponges. In order to improve the properties of these macromaterials, however, we must understand the behavior of CNTs in solution.CNTs can be dissolved in chlorosulfonic acid (CSA) and create a liquid crystal phase at high concentrations. At intermediate CNT concentrations, the liquid crystal phase forms droplets known as tactoids which float freely in the more dilute isotropic phase. The alignment of CNTs inside tactoids, classifies the type of liquid crystal phase as nematic or smectic. So far, tactoids formed in CNT-CSA solutions are characterized as nematic. Here, we show that tactoids formed in solutions of purified CNTs display a rippled texture on the surface with a spacing of about 2 µm.

UG-15   Visible-light two-photon excitation for subtractive SAX imaging

Katelyn Miyasaki,[1,2] Ryosuke Oketani,[3] Toshiki Kubo,[3] and Katsumasa Fujita[3]
[1]*Department of Biomedical Engineering, Washington University in St. Louis, St. Louis, MO, USA*
[2]*Nakatani RIES: Research and International Experiences for Students Fellowship in Japan, Rice University, Houston, TX, USA*
[3]*Department of Applied Physics, Osaka University, Suita, Osaka, Japan*

Techniques for imaging beyond the diffraction limit, especially those that do not damage cells and can image multiple targets simultaneously, are particularly relevant to viewing biological processes. Since no perfect imaging technique exists, scientists continue to optimize imaging processes for different situations. Many of today's super-resolution imaging techniques rely upon nonlinear relationships in fluorescence emission. We are combining two techniques for super-resolution fluorescence imaging, subtractive saturated excitation (SAX) microscopy and visible-light two-photon excitation (2PE), in order to ascertain the level of detail that can be obtained. To this end, we developed an optical system to acquire scanning fluorescence images and obtained fluorescence curves for fluorescent proteins to confirm 2PE. Then, we imaged a number of different samples, including fluorescent beads and cells containing fluorescent protein tags. Using these images, we produced subtractive images in search of a nonlinear response that would confirm the effectiveness of subtractive SAX. We expect to be able to surpass the resolution achievable with either subtractive SAX or visible-light 2PE alone through combining them, thereby improving biological microscopy studies.

UG-16   Exploring Zn-based Compounds for Visible Light Induced Photocatalysts

Emily Nishiwaki,[1,2,3] Daichi Kato,[4] and Hiroshi Kageyama[4]

[1]*College of Arts and Sciences, Cornell University, Ithaca, NY, USA*
[2]*Department of Materials Science and Engineering, Case Western Reserve University, Cleveland, OH, USA*
[3]*Nakatani RIES: Research and International Experience for Students Fellowship in Japan, Rice University, Houston, Texas, USA*
[4]*Department of Energy and Hydrocarbon Chemistry, Kyoto University, Kyoto, Japan*

The implications of climate change urge the need for efficient alternative energy sources such as H_2 gas. H_2 gas can be produced by reducing and oxidizing (splitting) of water; however, this process is thermodynamically unfavorable. Many catalysts already exist that can utilize UV light to assist in the splitting of water, but compounds that can utilize visible light, which have a band gap of less than 3.0eV, are still being developed. Mixed anion compounds, which often have small band gaps, have great potential to split water with visible light. In 2005, a ZnO-GaN solid solution adopting the wurzite structure was shown to have a band gap well below 3.0eV and exhibit a remarkable photocatalytic activity. This discovery led to extensive search for oxynitrides, but it is largely focused on perovskite type oxynitrides with octahedral coordination. We presume

that a polar structure is crucial to suppress undesirable electron-hole recombination. This research project aims to explore new oxynitrides that have a tetrahedral network, which lack 'local' inversion symmetry. Using high temperature ammonolysis reaction and high pressure reactions, we attempted to nitridize a $SrZnO_2$ oxide by Ga substitution to finally yield $Sr(Zn_{1-x}Ga_x)O_{1-x}N_x$. Other target compounds such as LaZnON and SrTiONF were also investigated.

UG-17   Gold Nanoparticles for the Ultrafast Control of Light

Andrea Schirato,[1,2] Alessandro Alabastri,[2] Peter Nordlander,[2] and Bruno Palpant[1]
[1]*Laboratoire de Photonique Quantique et Moléculaire, Ecole Centrale Paris, Paris, France*
[2]*Department of Physics and Astronomy, Rice University, Houston, Texas, United States*

A photonic crystal cavity represents an optical system that, owing to periodic sub-wavelength structures and induced defects, makes a strong localization of photonic modes possible. High electric field enhancements can be reached and an unusual concentration of energy is observed. In parallel, metal nanoparticles exhibit a resonant optical response sensitive to sub-picosecond time scale perturbations and are able to modify the optical properties of the effective medium. Furthermore, owing to their ultrafast responsivity, plasmonic nanostructures can absorb femtosecond light pulses, experiencing remarkable photo-induced modifications of their optical and thermal properties, provided that source electric fields are large enough. Thus, by coupling photonic crystal cavities and plasmonic systems, photo-induced media properties modifications become possible.

This study investigates the coupling in a hybrid plasmonic-photonic structure, in which gold ellipsoidal-shaped nanoparticles are embedded within a one-dimensional photonic crystal. The intrinsic geometric anisotropy of these nano-ellipses leads to a double resonance according to the polarisation of light. This property is considered as a promising degree of freedom with potential applications such as optical interconnects or switches.

Simulations show the possibility to achieve an ultrafast control on the transient optical behaviour of such a hybrid structure via the coupling of the two resonances. The system offers moreover a plethora of parameters that can be easily modified in the sample, leading to a relevant tunability of the optical response.

UG-18   Relation Between Phase Transition and Laser Irradiation Strength and Time Duration through Phase Patterning of MoTe₂

Trevor Shimokusu,[1,2] Kota Kamiya,[3] Nobuyuki Aoki,[3] and Jonathan Bird[4]

[1]*Department of Mechanical Engineering, The University of Hawai'i at Mānoa, Honolulu, Hawai'i, U.S.A*
[2]*Naktatani RIES: Research & International Experience for Students Fellowship in Japan, Rice University, Houston, Texas, U.S.A*
[3]*Graduate School of Advanced Integration Science, Chiba University, Inage-ku, Chiba, Japan*
[4]*Department of Electrical Engineering, University at Buffalo, The State University of New York, Buffalo, New York, U.S.A*

An intriguing property displayed by transition metal dichalcogenides (TMDCs) known as polymorphism, is attractive for its application in future electronic devices. Molybdenum ditelluride ($MoTe_2$) is a TMDC with an energy difference of ~35 meV between its semiconducting 2H and metallic 1T' phases, which is considerably less than the homologous energy differences of other TMDC materials [1,2]. By taking advantage of this smaller energy difference, we were able to feasibly observe polymorphism within $MoTe_2$. In this study, we fabricated $MoTe_2$ field effect transistors, and used laser-driven phase patterning to induce property changes in desired areas of the semiconducting channel [3]. While previous studies have confirmed successful 2H-1T' phase transition at laser irradiated sites, we investigate the possibility of controlling semiconducting properties

by controlling laser irradiation strength and time. We are particularly interested in p-n polarity and threshold voltage shifts (from normally-off to normally-on) of $MoTe_2$ upon phase patterning, as establishment of such relationships is essential for configuring electrical circuits within crystals of $MoTe_2$. Furthermore, we attempt to describe the mechanism behind the phase patterning induced phase transition. Although it is known that the formation of the Te-atom vacancy serves as the key origin for phase transition [3], the specific cause of this vacancy and other related causes of phase transition are still not confirmed. Realizing the previously stated relationships along with the driving mechanism of phase patterning opens the potential of fabricating circuit components, such as logic gates and transistors, with a uniform material.

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UG-19   Encapsulation of $MoTe_2$ nanoribbons inside carbon nanotubes

Shivani Shukla,[1,2] Yusuke Nakanishi,[2] and Hisanori Shinohara[3]

[1]*Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania, USA*
[2]*Nakatani RIES: Research and International Experience for Students Fellowship in Japan, USA*
[3]*Department of Chemistry & Institute for Advanced Research, Nagoya University, Nagoya, Japan*

Previous research has shown that the physical properties of bulk crystalline materials can vary greatly as the material is transformed from 3D-bulk to 2D-sheets or nanotubes, and finally to 1D-nanoribbons. Specifically, bulk graphite is conductive, as is single-layer graphene, but carbon nanotubes conduct electricity differently depending on chirality. Finally, graphene nanoribbons are semiconducting. A different pattern has been observed in transition metal dichalcogenide (TMD) nanoribbons, such as molybdenum disulfide. It is important to further study this interesting physical phenomenon in other TMDs and crystals, to uncover novel physics and eventually apply each nanomaterial optimally in future devices. Research has shown that high-yield synthesis of MoS_2 nanoribbons via encapsulation inside CNTs is difficult to achieve. In this study, we have successfully encapsulated $MoTe_2$ nanoribbons and tellurium nanowires inside CNTs via sublimation.

UG-20   Small Compounds and Microfluidic Culture for Inducing Maturation of hiPSC-derived Hepatocyte-Like Cells

Kaylene Stocking,[1,2] Nicolas Minier,[3] and Ken-Ichiro Kamei[4]

[1]*Bioengineering and Computer Engineering, University of Pittsburgh, Pittsburgh, PA, USA*
[2]*Nakatani RIES: Research and International Experience for Students in Japan Fellowship, Rice University, Houston, TX, USA*
[3]*Biomedical Engineering, Université Paris Descartes, Paris, Île-de-France, France*
[4]*Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University, Sakyo-ku, Kyoto, 606-8501 Japan*

Hepatocytes play a critical role in drug metabolism in the human body, and thus culturing these cells *in vitro* would allow for humane safety testing of new drugs. Instead of using human primary hepatocytes, causing human induced pluripotent stem cells (hiPSCs) to differentiate into hepatocyte-like cells (HLCs) is one method of obtaining cells for culture. Additionally, it is a promising treatment for liver disease. However, current methods have produced cells resembling fetal hepatocytes more closely than adult ones, and do not express enzymes critical for drug metabolism. We hypothesize that using 3D cell culture as well as incorporating tensile stress and small-molecule compounds into the culture environment might better mimic *in vivo* conditions and thus produce more mature HLCs from hiPSCs. To study 3D cell culture and chemical compounds, we introduce

six compounds to a microfluidic culture environment. These compounds are thought to play a role in signaling pathways related to hepatocyte differentiation and maturation. Of them, five have been used in other types of culture, while one is entirely new to differentiation research. Hepatocyte-committed hiPSCs at 16 days of growth are cultured in microfluidic wells with different combinations of the compounds added to a hepatocyte-growth basal medium. At day 22, cells are harvested and gene expression will be evaluated using immunocytochemistry and quantitative reverse transcription polymerase chain reaction (RT-PCR) to determine which compounds produce HLCs most similar to adult hepatocytes. We expect that the final results will help in further refinement of HLC maturation procedures.

UG-21 Investigation of carbon nanotube fiber strength after post-spinning fiber twisting

Xirui Wang[1], Oliver Dewey[1], Lauren Taylor[1], Matteo Pasquali[1][2]

1. Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas, United States
2. Department of Chemistry, Rice University, Houston, Texas, United States

The unique properties of carbon nanotubes (CNTs) mean they have a good combination of low density and high flexibility, as well as outstanding mechanical strength and electrical conductivity. Fibers made of CNTs bring these properties to the macroscopic level, making them an ideal multifunction material. In wet spinning fiber processing, CNTs are dispersed in chlorosulfonic acid (CSA) to produce the spinning solution (dope). The dope is extruded through a small orifice, forming a fiber filament to be collected on spinning drums as CNT fibers. The tensile strength of fiber samples is then measured by their breaking force under tension. Previous experiments have improved tensile strength mainly by varying spinning parameters and CNT types but did not fully consider post-spinning treatments as an alternative. The twisting of fibers likely packs more nanotubes in the same cross-sectional area, increasing the density which as shown by past research, improves CNT fiber strength. This study applies this hypothesis to investigate the correlation between the tensile strength and post-spinning twisting of CNT fibers at specific lengths. Initial tests showed that fibers twisted between 50 and 125 turns had electrical properties similar to the untwisted control samples, which is evidence of no additional misalignments after twisting. Further tests were performed to confirm the density changes of twisted samples by examining fiber diameter variations. Finally, the twisting of the samples was tested as a function of the breaking force to establish a correlation. This would present future CNT fiber production with an available post-spinning treatment for increasing fiber tensile strength.

UG-22 Encapsulation of Aluminum Nanocrystals @ Metal-Organic Frameworks

Daniel Weinberg[1,5] *, Hossein Robatjazi[2,5] *, Peter Nordlander[1,3,4,5], Naomi J. Halas[1,2,3,4,5]

[1] Department of Chemistry, Rice University, Houston, Texas, USA
[2] Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA
[3] Department of Physics and Astronomy, Rice University, Houston, Texas, USA
[4] Department of Material Science and Nanoengineering, Rice University, Houston, Texas, USA
[5] Laboratory for Nanophotonics, Rice University, Houston, Texas, USA

The incorporation of plasmonic metal nanoparticles into metal-organic frameworks (MOFs) has shown promise across a range of applications including photocatalysis, drug delivery, and gas storage. The large uniform pores in a MOF are particularly fascinating as the flexibility of MOF synthesis allows for rational design of pore size, shape, and chemical environment. Plasmonic @ MOF hybrid structures combine the optical properties of plasmonic nanoparticles with the selectivity gains due to molecular sieving in MOF pores. Thus far, plasmonic @ MOF structures have incorporated only noble/coinage metal nanoparticles. Aluminum

nanocrystals (Al NCs) display excellent optical properties using cheaper and more abundant materials, but the potential for plasmonic aluminum @ MOF structures has not yet been explored. The challenge posed by these Al NCs is the oxide layer that quickly forms upon exposure to air. The amorphous nature of this layer makes it poorly suited to traditional MOF nucleation and growth. In this work, we describe a strategy for the encapsulation of Al NCs in MOF coatings that adapts to the unique task of Al NC functionalization by turning this oxide layer to our advantage. Using a dissolution-regrowth mechanism we utilize the Al(III) centers within the oxide layer to form the backbone of the growing MOF to afford a uniform MOF coating around every Al NC while maintaining the shape and plasmonic properties of the particles. The encapsulated particles show increased N_2 absorption and surface area as compared to pristine Al NCs.

UG-23   WSe₂ Thin-Film Growth by Molecular Beam Epitaxy and Electric Double-Layer Transistor Implementation

Joshua Yang,[1,2,3] Yuta Kashiwabara,[3] Yue Wang,[3] Masaki Nakano,[3,4] and Yoshihiro Iwasa[3,4]

[1]*Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, U.S.A.*
[2]*Nakatani RIES: Research and International Experience for Students Fellowship in Japan, Rice University, Houston, Texas, U.S.A.*
[3]*Department of Applied Physics, The University of Tokyo, Tokyo, Japan*
[4]*Quantum-Phase Electronics Center, The University of Tokyo, Tokyo, Japan*

In the past, transition metal dichalcogenides (TMDCs) have been widely studied for their bulk-form applications as semiconductors, with an indirect bandgap in the near-infrared spectral range. More recently, however, there has been a surge in interest towards TMDCs, with a new focus on thin films and monolayers instead. In monolayer form, TMDCs (like WSe₂) have direct bandgaps in the visible spectral range and display photoluminescence of up to four orders of magnitude greater than in their bulk counterparts.[1] This allows for many novel applications in devices like FETs, LEDs, sensors, and even photovoltaic solar cells. While there are many different methods to synthesize and fabricate TMDC films, including, but not limited to, mechanical exfoliation, liquid exfoliation, and chemical vapor deposition, molecular beam epitaxy (MBE) is a bottom-up method that has greater potential for scalability in industry and is capable of producing large uniform crystals on the millimeter scale. To demonstrate the viability of MBE-grown films, we grew both multilayer and monolayer WSe₂ films by MBE on various substrates. Sapphire, SiC, and mica were chosen for their atomically smooth surfaces, and SiO_2 and $SrTiO_3$ were chosen for their potential uses as back-gate dielectrics in electronics. Characterizing the film with x-ray diffraction and Raman spectroscopy, we then selected the highest quality films for fabrication in an electric double-layer transistor, measuring the resulting transport characteristics using a Physical Property Measurement System (PPMS®). By examining substrate-dependent MBE film growth quality, we hope to spur on and expand the field of future 2D TMDC research.

[1]Wang, Q. H., Kalantar-Zadeh, K., Kis, A., Coleman, J. N., & Strano, M. S., *Nature Nanotech.* **7**, 699–712 (2012).

UG-24   Polarized Photoluminescence Excitation Spectroscopy of Aligned (6,5) Carbon Nanotubes

Jorge Zepeda O[1,2], Fumiya Katsutani[1] and Junichiro Kono[1,2,3]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA*
[2]*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*
[3]*Department of Materials Science and NanoEngineering, Rice University, Houston, Texas 77005, USA*

Photoluminescence excitation (PLE) spectroscopy is a strong tool to optically explore many of the properties of one-dimensional materials. Due to the van Hove singularities present in single-wall carbon

nanotubes (SWCNTs), only photons with certain energies can excite the SWCNTs and cause emission. Employing PLE, we are able to identify these peaks in excitation, and hence identify the species of SWCNTs by this spectral signature. Further, by creating a film of aligned SWCNTs, we can use polarized PLE in order to observe angular dependence allowing us to deduce the alignment quality of the film. Here, after optimizing the PLE setup, we analyzed polarized PLE data collected from (6,5) SWCNTs in solution and partially aligned on a film. The solution demonstrated a sharp peak of excitation near 2.18 eV with emission near 1.26 eV. Further, a second emission peak was observed near 1.11 eV with similar excitation energy – likely caused by defects in the sample. In contrast, the film demonstrated a peak of excitation near 2.14 eV with emission starting near 1.22 eV and slowly decaying until 0.92 eV. The fact that we did not observe a strong peak as expected, but a peak with a long tail is largely attributed to disorder and tube-tube interaction in the highly packed SWCNT film. Still, polarized PLE data showed that an angular dependence exists, which allows us to estimate the degree of alignment in the film as well as any modification to the polarization selection rules due to intertube coupling

UG-25   Insulation of Doped Carbon Nanotube Fibers at Elevated Temperatures

David Zhou[1], Oliver Dewey[1], Lauren Taylor[1], and Matteo Pasquali[1,2]

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

Carbon Nanotubes (CNT) have long been known for their impressive thermal conductivity, mechanical strength, and electrical conductivity. Using a solution spinning process, CNTs are formed into neat, macroscopic fibers with excellent properties similar to the single molecule in a more useful form for application-based work. However, CNT fibers exhibit lower electrical conductivity than single molecules and need to be improved for industry use. Electrical conductivity can be enhanced through the use of dopants such as iodine and other halogens, acids such as chlorosulfonic acid, and organics such as tetracyano-p-quinodimethane. However, when put under high temperatures doped CNT fibers are susceptible to decreased performance due to dopants diffusing out of the fiber. One method to minimize dopant loss is by coating with an impermeable layer to trap the dopant in the CNT fiber and allow for high electrical conductivity at elevated temperatures. Critical variables to consider are the electrical resistance of the coating, thickness of this insulator, the type of insulator used, and the dopant used. This research presents a method to test electrical conductivity as a function of temperature. This method uses a CNT fiber strung along an insulating substrate with 4 small metal leads soldered onto the apparatus in the usual positions of a 4-point probe. The device is then clamped down at the location of the leads for improved electrical contact with the fiber and placed in an oven. Preliminary results showing the performance of parylene as a coating will be presented, with future experiments focused on PEEK, Kevlar, and Nomex coatings.

UG-26   Determination of Aromatics and Resins in Crude Oils

David Valdes[1], Rocio Doherty[1]

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

Accurately quantifying and separating components of crude oils has shown to be cumbersome due to the four different fractions of oil: saturates, aromatics, resins, and asphaltenes. Each component is more complex and varied than the next, which results in accurate analysis being skewed. Asphaltene precipitation leads to detrimental safety issues and thousands of dollars lost in the removal of the solids. The biggest safety concern that follows asphaltene precipitation is the possibility of plugging safety devices/valves that, when fail to open or close, lead to adverse effects (Sunil L. Kokal and Sunil L. Kokal 1995). Acquiring a proper technique to

analyze crude oil fractions, especially resins, aromatics, and asphaltenes (Leontaritis, K.J. and Mansoori, G.A 1988), is essential to comprehending how each crude oil component affects precipitation and how we can prevent it. Resins and aromatics are neither volatile nor able to aggregate through precipitation, therefore a consistent method to fractionate and quantify them is difficult to obtain. Through separation procedures, such as evaporation, precipitation, and high performance liquid chromatography (HPLC), we can accurately separate and quantify each component of crude oil samples. Using the HPLC as our main method of separating aromatics and resins, we are able to sum the components masses to then quantify weight percentages of each component. We have been able to accurately quantify asphaltenes and volatile saturates through deposition and evaporation respectively. In this work, we propose a methodology to separate and quantify the amount of resins and aromatics by HPLC.

RSTEM UG Poster Session Participants

RSTEM-REU-01   Microfluidics in the study of *Hydra vulgaris'* nervous system

Darielys Prado Hernandez[1], Krishna N. Badhiwala[2], Daniel L. Gonzales [3,4], Jacob T. Robinson[2-5]

[1]*Research Experience for Undergraduates Program, Rice University, Houston, TX, USA*
[2]*Bioengineering, Rice University, Houston, TX, USA*
[3]*Applied Physics Program, Rice University, Houston, TX, USA*
[4]*Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[5]*Neuroscience, Baylor College of Medicine, Houston, TX, USA*

Microfluidic technologies are a powerful tool to study the nervous system of small model organisms. The cnidarian *Hydra* is a great model for neuroscience because of its distributed nerve net with reduced number of spiking neurons. Despite lack of complex sensory organs, it has shown to be able to perceive a change in its environment. In fact, it has been revealed before that *Hydra* is more responsive to blue light by increasing its periodic activity. To better study the behaviors of the freshwater jellyfish, *Hydra vulgaris*, we are using microfluidic technologies to precisely manipulate its environment. Here we show how changes in factors like lighting conditions, temperature, and the presence of chemicals can alter rate of body contractions. The anticipated outcome of this investigation, respecting the change in temperature, is that *Hydra* is likely to exhibit normal contraction activity at the temperature it was raised at and prefer to occur the space at that temperature.

RSTEM-REU-02   Optimizing the Characterization of Carbon Nanotubes

Jamie John Mana-ay,[1] Francesca Mirri,[1] Lauren Taylor,[1] and Matteo Pasquali[1]
[1]*Chemical Engineering, Rice University, Houston, Texas, United States*

Optimizing the purification process has always been a fundamental challenge to obtaining high quality carbon nanotubes (CNTs). This problem stems from the fact that when CNTs are initially produced, impurities such as amorphous carbon and catalyst elements are present in the reaction products. To remove the impurities CNTs must be subjected to thermal oxidation; however, this process can shorten CNTs. Because both purity and length are essential to make high quality materials, the purification temperature and time must be optimized to obtain relativity long and pure CNTs. To determine the optimal combination, a control sample was prepared, different thermal oxidation and exposure parameters were explored and a series of qualitative and quantitative measurements to assess CNT length and purity were performed. The nematic transition concentration (onset of liquid crystalline phase) was found by dissolving CNTs in Chlorosulfonic acid. This measurement can give an

estimate of the CNT length. In addition, the weight lost after oxidation was determined to assess the CNT purity. Finally, extensional rheology was used to estimate the aspect ratio (length over diameter of CNTs), and Raman spectroscopy to obtain the G to D ratio which is correlated to sample purity.

RSTEM-REU-03   Expanding EsaR N-Acyl Homoserine Lactone Signal Recognition Capability

Nancy Licona,[1] Joanne Ho,[2] and Matthew Bennett[2][3]
[1]*Office of STEM Engagement, Rice University, Houston, TX, USA*
[2]*Department of Biosciences, Rice University, Houston, TX, USA*
[3]*Department of Bioengineering, Rice University, Houston, TX, USA*

Quorum sensing (QS) is used by bacteria as a communication signaling mechanism to modulate bacterial behavior in proportion to cell density. The transcriptional regulatory protein EsaR binds to QS signaling molecules to induce gene expression. However, EsaR only recognizes the signaling molecule N-hexanoyl-L-homoserine lactone (C6HSL). The purpose of this study is to engineer EsaR to recognize an expanded set of N-acyl homoserine lactone signals, *i.e.* C4HSL, C6HSL, C8HSL, C10HSL, C12HSL, and C14HSL. First, a fusion protein SdiA-EsaR was prepared through site-directed mutagenesis to generate a library of chimeras. Next, HSL sensitivity was tested and reporter gene expression was measured when the protein acts as a transcriptional activator, which occurs when the esa box, or operator, sequence is at the -20 position relative to the transcription start site. We used a non-continuous directed evolution technique called PANCE to generate and select for evolved SdiA-EsaR variants that are specific to each of the signaling molecules. Results for this study are yet to be determined. By expanding EsaR signaling sensitivity, the unique transcriptional characteristic of EsaR as a dual activator-repressor is retained and this tool can be used to engineer genetic circuits inside living cells.

RSTEM-REU-04   Image Dehazing with Dark Channel Prior

P. Griggs Hutaff,[1] Manoj Kumar Sharma,[2] and Ashok Veeraraghavan[2]
[1]*Office of STEM Engagement, Rice University, Houston, TX 77005, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX 77005, USA*

Capturing high quality images in the presence of scattering media poses a challenge for designers of imaging systems. Image hazing is the result of backscatter, which is ambient light scattered towards the imaging device. Atmospheric conditions such as rain and fog are common factors of hazing. Multiple techniques have been created to remove haze from a captured image. Most of these techniques exploit the fact that the measured intensity at each pixel is a function of the medium transmission/scattering properties, object radiance and global atmospheric light. Using an algorithm to solve for the unknown values, it is possible to then remove the effect of haze and compute a de-hazed image that has higher resolution and contrast. The goal of our project is to study, implement and demonstrate the performance characteristics of existing de-hazing algorithms.

RSTEM-REU-05   Study of the Physical Properties of Multidomain Peptide Hydrogels as Biomaterials for Tissue Regeneration

Lei Gonzalez[1], Tania López Silva[1], and Jeffery D. Hartgerink[1,][2]
[1]*Department of Chemistry,* [2]*Department of Bioengineering, Rice University, Houston, Texas, United States of America*

Self-assembling multidomain peptide hydrogels (MDP) are promising materials for tissue regeneration. Several peptide sequences have been developed for specific applications. The physical properties and formation of each peptide sequence are affected by its structure and other factors such as concentration, temperature, strain, and pH. The purpose of this study is to determine the critical sol-gel concentration, and to study the properties and limitations of the hydrogels in different environmental conditions, as well as the uniqueness of each variant. In this work, six different peptide sequences were studied: $K_2(SL)_6K_2$ (SL), $K_2(SL)_6K_2DWIVA$ (DWIVA), $K_2(SL)_6K_2GESPLKRQ$ (ESP), $K_2(SL)_6K_2GIKVAV$ (GIKVAV), $K(SL)_6KGVFDNFLK$ (TenC 1K), and $K(SL)_3RG(SL)_3KG-RGDS$ (SLac). To find the physical properties of each gel, several experiments were conducted to change the solution-gelation critical point, which is found using table-top rheology and oscillatory rheology. First, we studied the effect of the concentration of peptide within the hydrogel, ranging from 2wt% to 0.01wt%. Second, the temperature of the environment, and third, the pH of the hydrogel. Oscillatory rheology allowed for the quantification of the results from table top rheology and the determination of the storage and loss moduli of the gel at each concentration. Finally, we found the lowest concentration at which the peptide in the solution forms a beta-sheet structure using Circular Dichroism Spectroscopy. From these experiments, we found that each gel is unique, and has different limitations and properties that affect their solution-gelation critical point. Some are very strong, like DWIVA and GIKVAV, while others are very weak, like TenC 1K and SLac.

RSTEM-REU-06   **Constraints on Temperature of Diamond-Carrying Magmas**

Michael Dean, Chenguang Sun and Rajdeep Dasgupta
Department of Earth, Environmental, and Planetary Sciences,
Rice University, Houston, Texas, United States

A major host of diamonds on the Earth is kimberlite, a CO_2-rich ultramafic igneous rock. Temperatures of kimberlitic magmas are important for understanding diamond formation in the deep mantle and consequent transportation to the Earth's surface. However, these temperatures remain unclear due to the lack of proper geothermometers for CO_2-rich magmatic systems. It has been well known that the equilibrium of Fe-Mg between the early-crystalized phase, olivine, and its coexisting melt can be used as a thermometer to measure the magmatic temperature of igneous rocks, but the effect of CO_2 has not been systematically examined. To calibrate this effect we ran piston-cylinder experiments at 1 GPa and 1250-1350 °C and varied the concentration CO_2 in our starting compositions. Olivine was added into a synthetic carbonatite to aid the saturation of olivine crystals in the CO_2-rich melt. Graphite capsules were used to maintain the reduced condition during the run. The recovered samples were analyzed for major elements in olivine and quenched glasses using an electron microprobe. Utilizing our new experimental data together with those in the literature, we plan to calibrate the general expression for Fe-Mg exchange coefficient (K_D)

$$\log K_D = \log \frac{(X_{FeO}^{Ol})}{(X_{FeO}^{Liq})} \frac{(X_{MgO}^{Liq})}{(X_{MgO}^{Ol})} = A + \frac{B}{T} + f(x)$$

where X denotes the cation (Fe or Mg) content in olivine or melt; A and B are coefficients to be determined; T is temperature; and $f(x)$ is a function of melt composition including CO_2. This expression will then be applied to natural kimberlite samples to determine their magmatic temperatures.

RSTEM-REU-07   **Determining Posterior Signaling Pathways that Induce Neural Fates in Human Embryonic Stem Cells**

Lauren Crain,[1] George Britton,[2] and Aryeh Warmflash[2]

[1]*Office of Stem Engagement, Rice University, Houston, Texas, United States*
[2]*Biosciences Department, Rice University, Houston, Texas, United States*

The ectoderm differentiates into posterior neural fates under specific signaling conditions, however little is known on how the signals are spatiotemporally organized to direct posterior ectodermal patterning. For the differentiation of anterior ectodermal patterning, inhibition of TGFβ signaling form Sox2+ intermediate fates that are later subpatterned into anterior fates of neural, neural crest, placode, and epidermal tissue. Interestingly, in the formation of posterior fates, future neural ectoderm must first form neuromesodermal progenitor (NMP) intermediate fates before differentiating into neural fates. This project is oriented to better understand whether published signaling factors that form neuromesodermal intermediate fates are competent to be subsequently patterned into fates composed within the posterior ectoderm. Alternatively, a separate set of signals may be required to direct posterior ectodermal patterning that doesn't promote a neuromesoderm intermediate fate.

To determine the signaling conditions needed to upregulate GBX2 expression correlated with posterior fates, combinations of agonist and antagonists for RA, SB, Wnt, and FGF pathways were introduced. Currently, no GBX2 expression was detected in experimental or control groups. Varying levels of OTX2 and Brachyury expression were observed, leading to an assumption of a dysfunctional GBX2 antibody. Preliminary results suggest the activation of RA induces neural fates, but the conditions have yet to be determined.

Subsequently, we will determine the window to introduce BMP as a signaling factor to initiate gene expressions associated with various ectodermal fates. Lastly, this knowledge will be translated to micropatterned surfaces to observe GBX2 expression associated with posterior neural induction.

RSTEM-REU-08 The Innovation of a Novel Self-Healing Composite Material

Jacob Braden[1], Xinbo Wang[2], and Enrique Barrera[2]
[1]*Office of STEM Engagement, Rice University, Houston, Texas, United States*
[2]*Materials Science and Nanoengineering, Rice University, Houston, Texas, United States*

Even though spacecraft are able to detect and avoid larger objects in space, they can have issues doing so with the relatively smaller objects. These small objects move at very high speeds, so they have the ability to cause significant damage to the spacecraft. When damage is done to the spacecraft's shielding, it will usually need to be repaired; in order to provide a safe repair system, which can cover the entire pressure vessel, a self-healing, composite shielding is created. A carbon fiber weave is used in a Vacuum Assisted Resin Transfer Molding (VARTM) procedure to create composite panels. Then, Nomex aramid honeycomb structures are incorporated between the layers of carbon fiber reinforced composites; the purpose of the honeycomb structures is to provide the shielding more strength and to hold the self-healing material. A thixotropic gel, with relatively high strength and the ability to self-heal, is the chosen self-healing material for this project. It is theorized that the gel will improve the strength of the structure of the shielding, absorb some of the energy from projectile impacts, and most importantly, act as a self-healing agent for the shielding. Also, because gels have been shown to self-heal in a very short period of time, it is theorized that the gel will quickly seal any damage done to the shielding, which is very beneficial when working with pressure vessels. Characterization and testing results of the prototype design are forthcoming.

RSTEM-REU-09 Species Difference in Exploratory Behavior

Ogechukwu Anwaegbu[1], Madeline Burns[2], and Julia Saltz[2]

[1]*Office of Stem Engagement, Rice University, Houston, Texas, United States*
[2]*Biosciences Department, Rice University, Houston, Texas, United States*

Often times, it is assumed that higher learning ability within species should be ideal, but if higher learning ability is ideal and corresponded to better fitness, why is there a high proportion of variation between species and individuals within species? Learning is defined as a relatively lasting change in behavior that is as the result of experience. Current hypotheses have suggested that naive prior distribution, information from distant ancestors play an important role in species expression of exploratory behavior; further suggesting that genes may influence how an individual explores and processes information in the environment. There have been works that have associated exploratory behavior and learning, but more remains to be done to determine how the two are involved in a behavioral syndrome We will be studying how differences in habitat breadth influence exploratory behaviors within and between species. As well as, how differences in exploratory behaviors influence the learning process and lead to observable differences in learning. *Drosophila sechellia* and *Drosophila simulans* serve as a good model for this study because they are closely related and crossable, but they have significant differences in habitat breath. Through this, we will be able to begin to determine the association between personality and its influence on learning.

RSTEM-NEWT-REU-01 **Membrane Capacitive Deionization (MCDI) Optimization**

Sandra Gonzalez,[1] Oluwaseye Owoseni,[1] and Dr. Shane Walker[2]
[1] *Civil Engineering Department, University of Texas at El Paso, El Paso, Texas, USA*
[2] *Rice University, Houston, Texas, USA*

Membrane Capacitive Deionization (MCDI) is an existing desalination technology that uses potential difference across two porous electrodes to remove ions from solution. MCDI applications promises less energy consumption than conventional desalination methods such as reverse osmosis (RO). Tests were performed to show energy requirements, rejection, recovery for differential total dissolved solids (TDS) concentration for brackish water ranges. Other parameters varied for product and concentrate flow, and energy consumption include: detention time, voltage, and voltage applied. Results show low energy consumption but improvement is required for recovery and rejection

RSTEM-NEWT-REU-02 **3-D Printed Nanoparticle-templated Porous Nanomaterials for Water Treatment**

Carmen A. Chavez[1]; Andrew Pardo[1].; Juan C. Noveron [1]

[1] *Department of Chemistry, University of Texas at El Paso, El Paso, TX, United States*

Metal ion contamination of natural water sources is a major concern. Heavy metals such as Uranium pose threats to all living organisms exposed due to its chemical and radioactive properties. About 6 million residents in the United States are exposed to Uranium contamination in the water, warranting selective high-surface area absorbents of dangerous material. A 3D printable structure with integrated flow control incorporates nanocavities with selective binding of Uranium salts. Synthesis of copper-nanoparticles coated with acrylate molecules are photopolymerized into 3D structures using stereolithography to engineer the scaffold. Removal of the Cu NPs yields organic zeolites with nanoscale cavities capable of absorbing heavy metallic ions. Adsorbtion experiments have been done testing different ppm ratios of Sodium arsenate salt (Na_2AsO_4), comparing the efficiency of copper nanoparticles with the polymer and the imprinted cavities inside the actual polymer. The 3D design provides a tunable absorption capacity capable of handling different water flow rates without the application of an external force required.

RSTEM-NEWT-REU-03   **Graphene Oxide Coupled ZIF-67 in Polluted Fresh Water Solution**

Edgar Aldama[1], Karen Ventura[1], Dino Villagran[2]

Department of Chemistry, University of Texas at El Paso, El Paso, Texas 79968, United States

An efficient organic pollutant and common ions nano-adsorbent was developed using a Zeolitic Imidazolate Framework (ZIF) containing Co and Zn metals (ZIF-67). The prepared ZIF was used as a building block for three layer nanocomposites. Synthesis of the composites were developed by the successful preparation of the ZIF@GO and ZIF hybrid nanocomposites. The prepared adsorbents were used to remove methylene blue (MB) as a model for common organic pollutants and modeled fresh water was used for the removal of common ions. The adsorption capacity for each sample was measured using ultraviolet visible (UV-Vis) spectroscopy. These findings show that the newly developed adsorbents can remove organic pollutants, and simple ions better than MOF and GO nano-composites which makes them suitable candidates for water and wastewater treatments.

RSTEM-NEWT-REU-04   **Two-dimensional nanomaterial: Hexagonal Boron Nitride (h-BN) for anti-corrosive coating**

LaBree Dotson,[1] Weibing Chen,[2] and Jun Lou[2]

[1] *Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment REU Program, Rice University, Houston, TX, USA*
[2] *Department of Material Science and Nanoengineering, Rice University, Houston, TX, USA*

Flint's water crisis is evidence that corrosive water in pipelines without effective coating can cause severe corrosion, leading to toxic levels in drinking water of heavy metals such as nickel and chromium, dissolve in the water and could severely disturb the lives of residents and precipitate a social crisis. A common practice is to coat pipelines with chromium-containing materials to protect against corrosion, but this harmful to the environment because carcinogenic particles in chromium cause negative health impacts on aquatic animals. Hexagonal boron nitride (h-BN) is a single-layer material that has attracted researchers' attention due to its superior thermal conductivity, chemically inertness, hydrophobicity, and relative low cost in comparison to other two-dimensional materials. The objective of this research is to grow and functionalize h-BN on silicon wafer to facilitate large-scale growth and industrial applications. Chemical Vapor Deposition (CVD) was used to grow thin films of h-BN on a silicon wafer with a small amount of boron precursor. Furthermore, by crosslinking h-BN with other compounds via the functionalization of h-BN with a wet chemistry method, we obtained a material with a thinner physical structure and the formation of larger continuous flakes, which leads to a denser film after deposition, thus providing a more efficient anti-corrosive additive. Our data show growth of a substantial amount of raw h-BN and functionalization of exfoliated h-BN. We further characterized h-BN by Fourier transform infrared spectroscopy, Raman spectroscopy, Brunauer–Emmett–Teller analysis and scanning electron microscopy.

RSTEM-NEWT-REU-05   **Ion-Exchange Polymers Laced with Functional Solutes for the Improvement of Membrane Capacitive Deionization Performance and Selectivity**

Daniel Caña,[1] Amit Jain,[2] Jun Kim[3], Rafael Verduzco[2], and Qilin Li[3]
[1]*NEWT Research Experience for Undergraduates, Rice University, Houston, Texas, US*
[2]*Dpt. of Chemical & Biomolecular Engr., Rice University, Houston, Texas, US*

[3]Dpt. of Civil and Environmental Engr., Rice University, Houston, Texas, US

Interest and demand for membrane capacitive deionization (MCDI) research and development has increased steadily and substantially in recent years as a notably energy efficient method of water softening and desalination. However, controlled selective removal within mixed ion solutions in MCDI systems is challenging to achieve due to the behavioral similarity of hardness ions in the presence of co-ionic functional groups. Here we pursue an enhanced ion selectivity, reduced energy consumption, and improved adsorption efficiency of MCDI activated carbon electrodes through the addition of sodium alginate (Na-Alg) or chitosan solutes to the ion exchange polymer membrane. Certain poly(vinyl alcohol) (PVA) polymer ion exchange membranes laced with chitosan or Na-Alg solute were both deemed structurally suitable for MCDI applications and performance testing. The impacts of the Na-Alg and chitosan electrodes were examined via standard CDI testing to determine energy efficiency in addition to ICP-OES analysis to determine ion selectivity. Preliminary data for the chitosan coated electrodes taken during MCDI testing may indicate comparable salt removal performance to PVA coated electrodes that are absent of the additional solute.

RSTEM-NEWT-REU-06 **High-Strength Interconnected Three-Dimensional Biocomposite of Yeast and Two-Dimensional Materials**

Andy Bui,[1] Sruthi Radhakrishnan,[2] and Pulickel M. Ajayan [2]
[1]NEWT REU Program, Rice University, Houston, Texas, USA
[2]Department of Materials Science and Nanoengineering, Rice University, Houston, Texas, USA

Due to a variety of physical and chemical properties, unique, two-dimensional (2D) materials like hexagonal boron nitride (h-BN) and graphene show potential in practical applications in nano-electronics, optoelectronics, sensors, batteries and supercapacitors. However, translation of these properties to three-dimensional (3D) architecture is still challenging, particularly in creating a hard and firm structure. We demonstrate a new approach to produce 3D structures of layered materials utilizing yeast as structural support. During the process, yeast intercalates between the layers of materials to successfully exfoliate h-BN, and graphite. The resulting 3D exfoliated hBN/yeast and exfoliated graphite/yeast form clay-like, highly malleable solids with interconnected architecture. The clay can be heated to harden into high-strength composites. This is a simple, low-cost, scalable method that might be applicable to a wide range of 2D materials. These biocomposites show promise for transforming layered materials into new functional 3D solids, as well as the possibility of 3D-printing 2D materials into highly complex and efficient structures.

RSTEM-NEWT-REU-07 **Needleless Electrospun Membranes of Layered Double Hydroxide for Removal of Selenium in Wastewater**

Tanner Rosenthal[1], Mark Weller[2], Candace Chan[2]

[1]NEWT REU Program, Arizona State University, Tempe, Arizona, United States
[2]Materials Science and Engineering, School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, Arizona, United States

High surface area to volume membranes are ideal for the removal of contaminants in water. An emerging method to form such membranes from polymers is via electrospinning. Electrospinning is known generally to have a slow production rate; to overcome this, a needleless electrospinning setup was used to increase productivity. For this work, poly(vinylpyrrolidone) (PVP) was utilized to form nanofibers, with diameters ranging between 200-400 nm. Layered double hydroxides (LDH) have been shown to be a promising

sorbent for removing both oxoanionic forms of selenium (Se^{4+} and Se^{6+}). Herein, $Mg-Al-CO_3$ based LDH nanofiber composites were synthesized via electrospinning, both by incorporating pre-made LDH into the polymer solution before spinning, and by precipitation and growth from Mg and Al salts included in the polymer solution followed by in situ formation of LDH from exposure to sodium hydroxide. Due to the solubility of PVP in aqueous solutions, a facile ultraviolet crosslinking step was incorporated before immersion of as-spun nanowires in solutions, resulting in an insoluble LDH-incorporated membrane. The membranes have shown promising results after conducting a batch test. This novel method has potential for easily forming non-toxic, inexpensive membranes for future water treatment applications for a variety of contaminants.

RSTEM-NEWT-REU-08   **Recovery Limit Identification and Inorganic Fouling Characterization in Direct Contact Membrane Distillation**

Skyler Henry,[1] Charles Dahill,[2] Ana Barrios,[2,3] and François Perreault[2,3]

[1]*NEWT REU Program, Arizona State University, Tempe, AZ*
[2]*NEWT RET Program, Arizona State University, Tempe, AZ*
[3]*Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment, Arizona State University, Tempe, AZ*
[4]*School of Sustainable Engineering and the Built Environment, Arizona State University, Tempe, AZ*

Membrane distillation (MD) is a desalination technique that uses a temperature gradient across a hydrophobic, microporous membrane that allows water to evaporate through its pores and condense on the other side. This research seeks to determine how the water recovery by an MD process is limited by the formation of inorganic species that block the pores of the membrane and increase the feed water's resistance to flow. This information will give better insight into the scaling process so that future scaling prevention and reversal procedures can be developed. The general procedure includes identifying the recovery limit for a brackish oil and gas produced water by monitoring permeate flux during recovery, characterizing the membrane fouling using scanning electron microscopy coupled with energy dispersive X-ray spectroscopy, optical coherence tomography, and ion chromatography, and modelling the change in bulk solution chemistry through the equilibrium modeling program Visual Minteq. We found that permeate flux decline is dependent on both the initial ion concentration of the feed water and recovery time. In addition, equilibrium modeling has shown that the majority of foulants nucleated on the membrane are expected to be comprised of carbonate, sulfate, and calcium, and the elemental analyses support this expectation. Future research should address whether the threshold for recovery is dependent on membrane properties or temperature difference. These findings can also be used to compare inorganic fouling in traditional MD to that of solar MD.

RSTEM-NEWT-REU-09   **Pilot Scale Evaluation of Chitosan-Copper-Titanium Dioxide Media for Arsenic Removal from Water**

Chris De La O[1], Ariel Atkinson[2], Lauren Pincus[3], Julie Zimmerman[3], Paul Westerhoff[2]

[1]*NEWT REU Program, Arizona State University, Tempe, Arizona, USA*
[2]*School of Sustainable Engineering and the Built Environment, Arizona State University, Tempe, Arizona, USA*
[3]*School of Forestry and Environmental Studies, Yale University, New Haven, Connecticut, USA*

Arsenic is a carcinogen found in drinking water that must be removed before consumption. Zimmerman et. al. developed an innovative medium to selectively remove arsenic, nicknamed Zimmermedia. This medium is synthesized from titanium dioxide, copper oxide, and chitosan, which is a byproduct of shellfish manufacturing. The overall objective of this study is to evaluate the removal capacity of arsenic by Zimmermedia, in comparison to Bayoxide® E33, the industry standard for removal of arsenic. NSF53 standard

arsenic challenge water, was run through a column containing media for 7 days, and water constituents were measured daily in the influent and effluent. Separate column tests were performed for arsenic(V) and arsenic(III). During the arsenic(III) test, the column bed was under continuous UV light exposure, and no UV light was used in the arsenic(V) test. Constituent analysis of the effluent in comparison to the feed tank showed that Zimmermedia breakthrough occurred instantaneously under tested conditions.

RSTEM-NEWT-YS-01 **Improving Membrane Capacitive Deionization Using Composite Electrodes**

Cierra Weathers,[1] Amit Jain,[2] Jun Kim,[3] Qilin Li,[3] and Rafael Verduzco[2]

[1]*NEWT Young Scholars Program, Rice University, Houston, Texas, United States*
[2]*Dpt. of Chemical and Biomolecular Engr., Rice University, Houston, Texas, United States*
[3]*Dpt. of Civil and Environmental Engr., Rice University, Houston, Texas, United States*.

MCDI, or Membrane Capacitive Deionization, is a promising method developed to desalinate water through the removal of ions using a pair of activated carbon electrodes, each coated with an ion exchange membrane. Currently, activated carbon electrodes are created by preparing sheets with a slurry of powdered activated carbon and polyvinylidene difluoride binder. The desalination performance of such electrodes could be improved by using a hydrophilic binder (polyvinyl alcohol) and incorporating ion exchange polymers (sulfonated and aminated) into the activated carbon matrix. A composite slurry of these polymers and the activated carbon were prepared and flow-coated onto graphite sheets producing electrodes in a simple and scalable manner. These electrodes were then tested in the MCDI cell using NaCl as a feed solution, and their performance was evaluated based on four parameters: average salt absorption rate, salt absorption capacity, salt removal efficiency, and charge efficiency. The performance of the composite electrodes was superior to the standard flow-coated electrodes. Uniform surface morphology was observed using a scanning electron microscope FE-SEM, while the functional group structure was analyzed using a FTIR. Additionally, mixed salt tests were conducted using a mixture of NaCl and $CaCl_2$ as a feed solution. Slight ion selectivity was found for Na+ (effluent samples were analyzed through ICP-OES testing). The lack of ion selectivity was due to a lack of functional groups present in the slurry (analyzed through FTIR). Composite electrodes with increased functional groups could optimize salt removal efficiency and ion selectivity, therefore greatly improving the performance in the future.

RSTEM-NEWT-YS-02 **Degradation of 1,4-dioxane at Low Concentrations using Gram-Positive and Gram-Negative Mycobacteria From Two Bacterial Consortia Enriched In Uncontaminated Environments**

Aurian R. Maleki[1], Ya He[2], Pedro J. Alvarez Ph.D[2]

[1]*NEWT Young Scholars Program, Rice University, Houston, TX, USA*
[2]*Civil and Environmental Engineering, Rice University, Houston, TX, USA*

In the world today, manufacturing and polishing leads to extensive use of chemicals that pose a risk to global water supplies. One of these volatile chemicals, 1,4-dioxane, is a highly miscible groundwater contaminant proven to be a probable human carcinogen. Although dioxane can be removed through bacterial biodegradation, the process is partially ineffective at low concentrations of dioxane. In this study, we evaluated the potential of dioxane removal at low concentrations by two consortia enriched and sampled from uncontaminated garden soil samples with the abundance of bacteria, and we monitored the change in

concentrations over time. In the process of our research, we also used groundwater from a dioxane-contaminated site in Seattle, WA to mimic the contaminated environmental conditions and conducted biodegradation experiments by amending 20 mg/L bacterial biomass from two enriched consortia. We found that the two consortia can degrade dioxane to a non-detectable level (<5 μg/L). In later experiments, we discovered that the 16S rRNA gene sequencing shows that the dominant genus in the two consortia is *Mycobacterium*. Soluble diiron monooxygenase (SDIMO) gene sequencing also shows that group 5 and 6 SDIMO genes are involved in the degradation of dioxane. This study bolstered our understanding of dioxane degradation at low concentrations and the corresponding genetic study would facilitate us to develop biomarkers to assess the degradation potentials in impacted sites and create future innovations that can degrade large volumes of water.

RSTEM-NEWT-RET-01   **Scaffolding Collaboration of Middle School and High school teachers and students of water filtration with the use of nanotechnology.**

Claire Cook[1], Adam Carberry, Ph.D.[2], Meredith Morrissey [3]

[1]*NEWT Research Experience for Teachers, Arizona State University, Tempe, AZ, USA*
[2]*Engineering and Manufacture Engineering Program, Arizona State University, Tempe, AZ, USA*
[3] *Mountain Pointe High School Environmental Science teacher and RET NEWT 2016 intern, Phoenix, AZ*

Opportunities to build on content from one grade level to another is almost impossible. Rarely is there collaboration within a school among same subject teachers much less from one school to another. This opportunity allows for such an experience and the goal is to educate about water importance and nanotechnology. Centennial Middle School is located in Phoenix, AZ and its feeder high school is a mere 2 miles away where environmental science teacher Meredith Morrissey works and who couldn't wait to jump on the opportunity to collaborate. Using a water filtration activity in sixth grade where students engineer a filtration system that filters "bacterium", colored water, the high school students are doing something similar, but the difference is an enhanced filtering system using nanotechnology, specifically silver nitrate. The project is three fold: understanding clean water scarcity globally, understanding engineering and physically creating and testing their own filtration system, and lastly understanding nanotechnology and its importance within water filtration. Separately the students will learn these three aspects but together the collaboration and scaffolding occurs when the high school students come to the middle school to teach and explain the importance of the enhanced filter and in turn the middle schoolers can share their filters and results and together, they can compare and contrast both types of filters and which did a better job of eliminating the "bacterium." Lastly, the young students gain a greater perspective of science beyond just their grade level. They get to make connections and see future possibilities.

O-3A.1 – Interactions between a palsmonic particle and transition metal coatings

Seyyed Ali Hosseini Jebeli,[1] Anneli Joplin[2], Eric Sung[2], Wei-Shun Chang, and Stephan Link

[1]*ECE Department, Rice University, Houston, Texas, USA*
[2]*Department of Chemistry, Rice University, Houston, Texas, USA*

Hybrid nanostructures made from a noble and a transition metal have promising potential as photocatalaysts because transition metals have oxidation potentials in a suitable range for important reduction reactions and noble metals can absorb light strongly and act as an optical antenna. Au-Pt nanostructures are a well-characterized example of noble-transition metal hybrids, providing an ideal model for study of their fundamental optical properties. While the applications are vast for these types of nanostructures, the reason behind their increased photocatalytic activity is not yet fully understood. The proposed mechanisms range from near field enhancement by Au that results in increased absorption in Pt to hot carrier injection from Au to Pt that promotes reduction reactions on the Pt surface. In this work, we present correlated dark-field scattering, photoluminescence, and absorption measurements of single Au-Pt nanorods to evaluate the likelihood of these mechanisms based on their detailed optical properties. FDTD simulations were utilized to explain features observed in the experimental spectra. These simulations suggest that Au increases the absorption in Pt through field enhancement, which is amplified by the large imaginary part of the permittivity of Pt. Despite the increased absorption rate in Pt, however, absorption in Au itself is damped resulting in reduced radiative relaxation of hot carriers in the Au nanorod, and consequently lower photoluminescence signal. These findings will make it possible to design better structures for field enhancement and absorption and also to choose the best material for efficient photocatalysis.

O-3A.2 – Detecting the FFLO phase in an spin-imbalanced Fermi gas

Yi Jin, Jake A. Fry, Anna L. Marchant, Melissa C. Revelle, Randall G. Hulet

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas 77005*
[2]*Rice Center for Quantum Materials, Rice University, Houston Texas 77005*

The exotic Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) magnetized superconductor exhibits both superconducting and magnetic order. It occupies a large region of the one-dimensional (1D) phase diagram. However, the FFLO phase is more robust against quantum and thermal fluctuations in higher dimensions. This motivated us to map the dimensional crossover between 1D and 3D, as it is predicted to be the optimal regime to search for FFLO. We prepare a spin-imbalanced Fermi gas of lithium-6, analogous to creating a magnetized atomic cloud. By using a 2D optical lattice, we confine the atoms to 1D tubes and bring the system to the dimensional crossover regime by tuning the inter-tube tunneling rate and interaction strength. We take 1D time of flight measurements using a blue-detuned anti-trapping beam to cancel the axial confinement of the optical lattice. We look for signatures of FFLO in the time of flight spin densities.

O-3A.3 – How to Identify Plasmons from the Optical Response of Nanostructures

Runmin Zhang,[1] Luca Bursi,[2,3] Joel D. Cox,[4] Yao Cui,[1,5] Caroline M. Krauter,[6] Alessandro Alabastri,[1] Alejandro Manjavacas,[7] Arrigo Calzolari,[3] Stefano Corni,[3,8*] Elisa Molinari,[2,3] Emily A. Carter,[9] F. Javier García de Abajo,[4,10] Hui Zhang,[1] and Peter Nordlander[1]

[1]*Laboratory for Nanophotonics and the Department of Physics and Astronomy, MS61, Rice University, Houston TX 77005, USA*

[2]*Dipartimento di Fisica, Informatica e Matematica-FIM, Università di Modena e Reggio Emilia, I-41125 Modena Italy*
[3]*Istituto Nanoscienze, Consiglio Nazionale delle Ricerche CNR-NANO, I-41125 Modena, Italy*
[4]*ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain*
[5]*Department of Chemistry, Rice University, Houston TX 77005, USA*
[6]*Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544-5263, USA*
[7]*Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131, USA*
[8]*Dipartimento di Scienze Chimiche, Università di Padova, I-35131 Padova, Italy.*
[9]*School of Engineering and Applied Science, Princeton University, Princeton, NJ 08544-5263 USA*
[10]*ICREA-Institució Catalana de Reserca i Estudis Avançats, Passeig Lluís Companys 23, 08010 Barcelona, Spain*

In the past few years, plasmonics with the size of a few nanometers raised much interest, which enables the control over light-matter interaction at extreme-subwavelength scales. However, in this limit, quantum-mechanical effects strongly influence the plasmonic response, making it different from classical predictions. For small systems, collective plasmonic modes are hard to distinguish from other optical responses such as single-electron transitions. In this work, with the Random Phase Approximation method, we describe the basic properties of plasmonic reponses. Moreover, we define a universal metric for such classification, the generalized plasmonicity index (GPI), which can be easily implemented in any computational electronic-structure method or classical electromagnetic approach to discriminate plasmons from single-particle excitations and photonic modes. Our study offers a rigorous foundation for the further design of ultra-small nanostructures based on the molecular plasmonics.

O-3A.4 – **Photoinduced force mapping of plasmonic nanostructures**

<u>Thejaswi Tumkur</u>,*[1] Xiao Yang*[1,2], Chao Zhang,*[2] Ben Cerjan[2], Isabell Thomann[1,3,4,5], P. Nordlander[2,4], N. J. Halas[1,2,3,4,5]

[1]*Department of Electrical and Computer Engineering,*[2]*Department of Physics and Astronomy,* [3]*Department of Chemistry,*[4]*Laboratory for Nanophotonics,and* [5]*Rice Quantum Institute, Rice University, Houston, TX 77005 USA*
Equal contribution

Nanophotonic systems such as plasmonic structures, metamaterials and 2-D materials enable the control of several optical and chemical phenomena such as spontaneous emission, Raman scattering and catalysis, paving the way for a wide range of applications. The optical properties of such materials depend on the morphology of the constituents that make up the bulk structures. Consequently, it is imperative to understand the correlation between morphology and near-field optical properties with a high spatiotemporal resolution. In this work, we demonstrate the ability to map the forces between an optically excited sample and a tip, using a tool that combines atomic force and scanning probe microscopies. We show that the enhancement of near-field optical forces in gold disk dimers and nanorods are polarization sensitive and correlate well with expected plasmonic field enhancements. In a different set of experiments, we image the mutual interactions (hybridization) of individual gold-aluminum plasmonic heterodimers by mapping the spectral response of photoinduced forces and compare them to far-field extinction measurements. All our experimental results are complemented by calculations which estimate the forces between an optically excited sample and a nanoscale tip (in a realistic geometry). We believe that photoinduced force mapping will be a valuable addition to the toolbox of existing techniques for near-field imaging and characterization, enabling the study of fundamental physical and chemical phenomena.

O-3A.5 – **Protein transport dynamics at polymeric interfaces: A single molecule study**

Nicholas A. Moringo,[1] Hao Shen,[1] Lawrence J. Tauzin,[1] Wenxiao Wang,[2] Logan D.C. Bishop,[1] and Christy F. Landes[1]

[1]*Department of Chemistry, Rice University, Houston, Texas, U.S.A.*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, U.S.A.*

Tuning protein interactions at polymeric interfaces is essential to the efficacy of biomedical implants, food packing materials, and industrial protein purification processes. Functionalization is often utilized to introduce application specific surface chemistries to the outermost layer of a polymer, keeping the bulk polymer properties unchanged. Studying the adsorption of a protein at a polymeric interface with traditional ensemble based techniques provides little insight into the highly dynamic processes contained in protein-polymer interactions. Single molecule microscopy is a powerful in situ technique which provides high spatiotemporal movies of individual proteins interacting with polymeric interfaces. In this work single molecule microscopy is utilized to track the real time adsorption dynamics of lysozyme, a well-studied antibacterial protein, at the interface of polystyrene oxidized via UV exposure, oxygen plasma, and ligand grafting to produce varying degrees of surface hydrophilicity, surface roughness, and induced oxygen content. Tracking results indicate that lysozyme adsorption and surface mobility at the polymer interface is hindered as a result of all functionalization techniques. However, lysozyme adsorption dynamics depend on the extent of functionalization and the specificity of the oxygen moieties introduced to the polystyrene surface. Hindered adsorption and mobility is hypothesized to be dominated by hydrophobic effects attributed to water hydration layer formation at the functionalized polystyrene surfaces. These findings provide insight into determining application specific polymer functionalization techniques utilized in a wide array of polymer film applications.

O-3A.6 – **Unified Spin Model for Magnetic Excitations in Iron Chalcogenides**

Patricia Bilbao Ergueta,[1] Wen-Jun Hu,[1] and Andriy H. Nevidomskyy[1]

[1]*Rice University, Houston, Texas, USA*

Recent inelastic neutron scattering (INS) measurements on FeSe and $Fe(Te_{1-x}Se_x)$, have sparked intense debate over the nature of the ground state in these materials. Here we propose an effective bilinear-biquadratic spin model which is shown to consistently describe the evolution of low-energy spin excitations in FeSe, both under applied pressure and upon Se/Te substitution.

The phase diagram, studied using a combination of variational mean-field, flavor-wave calculations, and density-matrix renormalization group (DMRG), exhibits a sequence of transitions between the columnar antiferromagnet common to the iron pnictides, the non-magnetic ferroquadrupolar phase attributed to FeSe, and the double-stripe antiferromagnetic order known to exist in $Fe_{1+y}Te$. The calculated spin structure factor in these phases mimics closely that observed with INS in the $Fe(Te_{1-x}Se_x)$, series. In addition to the experimentally established phases, the possibility of incommensurate magnetic order is also predicted.

O-3B.1 – Synthesis and properties of fluorinated h-BN

Sruthi Radhakrishnan[1], Deya Das[2], Abhishek K. Singh[2], Pulickel M. Ajayan[1]

[1]*Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA-77005*
[2] *Materials Research Center, Indian Institute of Science, Bangalore, India-560012.*

In the midst of a number of ferromagnetic semiconductors such as tellurides and oxides, we explore the possibility of a stable two-dimensional (2D) wide bandgap insulator to be chemically and structurally modified into a magnetic semiconductor. The realm of 2D materials has emerged as promising new set of low-dimensional materials for semiconductor electronic devices. Chemical functionalization has been a known strategy to modulate and change the electronic properties of 2D materials. Here, we demonstrate a new approach to modify a 2D layered material, namely hexagonal boron nitride (h-BN), known for its structural, chemical and thermal stability, to create an unconventional semiconductor magnet, fluorinated h-BN (F-BN).

h-BN, a layered ceramic is an electrical insulator which on fluorination transforms into a wide bandgap semiconductor via introduction of defect levels. The electrophilic nature of fluorine cause changes in the charge distribution around neighboring nitrogen atoms in h-BN leading to room temperature weak ferromagnetism. The observations are supported by theoretical calculations considering various possible configurations of fluorinated h-BN structure and their energy states. This unconventional magnetic semiconductor material could spur studies of stable 2D magnetic semiconductors. While the high thermal and chemical stability of h-BN have found a variety of uses, this chemical functionalization approach expands its functionality to electronic and magnetic devices.

O-3B.2 – **Aluminum nanocrystals @ metal-organic frameworks core-shell structure: a new addition for sustainable plasmonics**

Hossein Robatjazi [1,5], Daniel Weinberg [2,5], Peter Nordlander[1,3,4,5], Naomi J. Halas[1,2,3,4,5]

[1] *Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*
[2] *Department of Chemistry, Rice University, Houston, Texas, USA*
[3] *Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[4] *Department of Material Science and Nanoengineering, Rice University, Houston, Texas, USA*
[5] *Laboratory for Nanophotonics, Rice University, Houston, Texas, USA*

Metal-organic frameworks (MOFs) are a class of materials with exceptionally high porosity and surface area consisting of a crystalline lattice of metal cations centers connected by anionic organic linker molecules which create complex networks of regular pores and channels. The synthesis and characterization of MOFs is one of the most rapidly developing areas of both chemistry and chemical engineering due to their enormous potential for practical applications such as heterogeneous catalysis. In this regard, incorporation of MOFs around plasmonic metal nanoparticles is a promising approach to enhance the efficiency in plasmon-driven photocatalysis due to improving the reactant uptake near the catalytic centers. In this work, we describe a facile strategy for the synthesis of aluminum nanocrystals (Al NCs) @ MOFs core-shell structure. Unlike noble/coinage metal nanoparticles, Al naturally forms a few-nm protective oxide surface layer that protects Al NCs from further oxidation. However, its amorphous nature is a barrier for further modification of the Al surface. The key for formation of an Al@MOF hybrid lies in turning the native oxide layer to our advantage by adopting a dissolution-regrowth mechanism of MOF formation. This approach utilizes Al(III) centers in the native oxide to form the backbone of the MOF, obviating the need to introduce an additional metal precursor to the reaction mixture. The flexibility of this present

strategy was demonstrated for uniform coating of Al NC cores with MOFs of differing pore size and structural geometry. The hybrid has shown drastically increased N_2 uptake and surface area compared to pristine Al NCs. The introduction of plasmonic@MOF structure based on Al NCs reaffirms the potential of Aluminum as alternative material to plasmonic noble/coinage metals for sustainable plasmonics.

O-3B.3 – **Ultrafast Dynamics of Single Aluminum Nanodisks**

Man-Nung Su[1], Pratiksha Dongare[2], Debadi Chakraborty[5], Yue Zhang[2,3], Chongyue Yi[1], Fangfang Wen[1], Wei-Shun Chang[1], Peter J. Nordlander[3,4], John E. Sader[5], Naomi J. Halas[1,3,4] and Stephan Link[1,4]

[1]*Department of Chemistry,* [2]*Applied Physics Graduate Program,* [3]*Department of Physics,* [4]*Department of Electrical and Computer Engineering, Laboratory for Nanophotonics, Rice University, Houston, TX 77005, USA* [5]*Department of Mathematics and Statistics, The University of Melbourne, Victoria 3010, Australia*

Aluminum nanostructures support tunable surface plasmon resonances and have become an alternative to gold nanoparticles. Whereas gold is the most-studied plasmonic material, aluminum has the advantage of high earth abundance and hence low cost. In addition to understanding the size and shape tunability of the plasmon resonance, the fundamental relaxation processes in aluminum nanostructures after photoexcitation must be understood to take full advantage of applications such as photocatalysis and photodetection. In this work, we investigate the relaxation following ultrafast pulsed excitation and the launching of acoustic vibrations in individual aluminum nanodisks, using single-particle transient extinction spectroscopy. We find that the transient extinction signal can be assigned to a thermal relaxation of the photoexcited electrons and phonons. The ultrafast heating-induced launching of in-plane acoustic vibrations reveals moderate binding to the glass substrate and is affected by the native aluminum oxide layer. In addition, we found an additional 30-ps relaxation corresponding to events happening at the core/shell metal/oxide interface. Finally, we increased the time resolution to sub-picosecond to study the initial dynamics of aluminum nanodisks. The sub-picosecond transient transmission is more responsive to lattice temperature than electron temperature.

O-3B.4 – **Synthetic dimensions in ultracold polar molecules: Quantum strings and membranes**

Bhuvanesh Sundar,[1,2] Bryce Gadway,[3] and Kaden R A Hazzard[1,2]

[1]*Department of Physics and Astronomy, Rice University, Houston TX 77005, USA* [2]*Rice Center for Quantum Materials, Rice University, Houston TX 77005, USA* [3]*Department of Physics, University of Illinois at Urbana Champaign, Urbana IL 61801, USA*

We show that rotational states of ultracold molecules can be used as a large synthetic dimension. Microwaves drive tunnelings between the synthetic lattice sites with a fully controllable magnitude and phase. For uniform synthetic tunnelings, we find that two molecules that are frozen in space and interact via a dipole interaction undergo two distinct binding-unbinding transitions in the synthetic dimension at critical interaction strengths. In a system with molecules frozen in a periodic array, the system undergoes a spontaneous dimensional reduction at the binding transitions, and collapses to a narrow strip in the synthetic direction. The resulting system is a quantum string (for a one-dimensional chain of molecules) or a membrane (for a two-dimensional array). At large interactions, an emergent strongly interacting condensate lives on the string or membrane. In a two-dimensional array of molecules, we also find evidence of a metastable non-Abelian Ising anyon phase. We show that these phases can be detected using measurements of rotational state populations.

O-3B.5 – Tilt Grain Boundary Topology Induced by Substrate Topography

Henry Yu,[1,2] Nitant Gupta,[2] Zhili Hu,[2] Kai Wang,[3] Bernadeta Srijanto,[3] Kai Xiao,[3] David Geohegan,[3] and Boris I. Yakobson[1,2]

[1]*Applied Physics Program, Rice University, Houston, TX, USA*
[2]*Materials Science & Nanoengineering, Rice University, Houston, TX, USA*
[3]*Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, USA*

Synthesis of two-dimensional (2D) crystals is a topic of great current interest, since their chemical makeup, electronic, mechanical, catalytic, and optical properties are so diverse. A universal challenge, however, is the generally random formation of defects caused by various growth factors on flat surfaces. Here we show through theoretical analysis and experimental demonstration that nonplanar, curved-topography substrates permit the intentional and controllable creation of topological defects within 2D materials. We augment a common phase-field method by adding a geometric phase to track the crystal misorientation on a curved surface and to detect the formation of grain boundaries, especially when a growing monocrystal "catches its own tail" on a nontrivial topographical feature. It is specifically illustrated by simulated growth of a trigonal symmetry crystal on a conical-planar substrate, to match the experimental synthesis of WS_2 on silicon template, with satisfactory and in some cases remarkable agreement of theory predictions and experimental evidence.

O-3B.6 – Quenching of Single-Walled Carbon Nanotube Fluorescence by Dissolved Oxygen Reveals Selective Single-Stranded DNA 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 O_2, 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.

Oral Session 4A: 3:30 PM – 4:45 PM

O-4A.1 – Mechanistic Understanding of the Formation and Evolution of the Nanoparticle Protein Corona: A Single-Particle and Single-Molecule Spectroscopic Study

Qingfeng Zhang,[1] Christy Landes,[1] and Stephan Link[1]

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

Nanotechnology holds great promise for many biomedical applications. However, the interactions of

nanoparticles with living systems is extremely complex and still poorly understood. If widespread application of nanomedicine is to be achieved, we must understand and control the complex and dynamic "protein corona" that forms upon nanoparticle incorporation by a living organism. The protein corona greatly affects nanoparticles' interactions with the physiological environment. My goal is to resolve the dynamics of the formation of the nanoparticle protein corona and follow its evolution over time using state-of-the-art single-particle and single-molecule spectroscopy, and subsequently to elucidate the underlying pathways in which the protein corona influences cellular uptake both *in situ* and *in vivo*. The knowledge gained through the proposed research would add significant new insights to the rational design of nanoparticles and their coatings including the *ex situ* rational design of a protein corona with a desired structure, composition, and surface functionality to enhance the nanoparticles' intended biological fate.

O-4A.2 – **Gadolinium-Filled Boron Nitride Nanotubes as MRI Contrast Agents**

Nicholas G. Zaibaq,[1] Sakineh E. Moghaddam,[1] Ricardo A. Rivera,[1] and Lon J. Wilson[1]

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

Boron nitride nanotubes (BNNTs) are structural counterparts of carbon nanotubes (CNTs), with distinct chemical and physical properties. BNNTs are a relatively unexplored material, with significant promising findings that they can be used in biomedical applications. In this work, we have explored the gadolinium loading capacity of BNNTs for use as contrast agents (CAs) for magnetic resonance imaging (MRI). We have established a method that increases the Gd loading capacity 2.5 times that of current reports without the need for prior covalent functionalization or oxidation. We were able to achieve a higher loading capacity with first chelating the Gd^{3+} ions and then loading them into BNNTs, increasing the possible intermolecular forces that keep the Gd sequestered in the tube. This new material with a higher Gd content without the need for oxidation prior to loading could serve as a means for enhanced contrast for magnetic resonance imaging (MRI) and as a vector for both imaging and therapeutic agents (termed "theranostic agent") in the same material for image-guided therapy applications. Further, if MRI can be used to track BNNTs *in vivo*, this will allow their biodistribution and biological effects to be studied in a non-invasive manner with high resolution. Future directions include challenging the material in biological media and measuring relaxivity values. We plan then to incubate the material with stem cells to determine uptake, cyctocompatability, and imaging efficacy of the Gd-loaded BNNTs.

O-4A.3 – **Plasmonic Nanoparticles Accelerate Laser Curing of Thermoset Epoxies**

Jian Yang,[1] Alessandro Alabastri,[1] Adam T. Roberts,[2] Matt E. Reish,[3] Henry O. Everitt,[4] and Peter Nordlander[1]

[1]*Laboratory for Nanophotonics and the Department of Physics and Astronomy, Houston, TX, USA*
[2]*Northrop Grumman, Redondo Beach, TX, USA*
[3]*Oak Ridge Institute for Science and Education, Oak Ridge, TN, USA*
[4] *Army Aviation and Missile Research, DeveloPMent, and Engineering Center, Redstone Arsenal, AL, USA*

The benefit of using nanoparticles to concentrate heat and accelerate curing of high temperature epoxies is demonstrated for laser-bonded composites. By shining nanoparticles at their localized plasmon resonance with a laser source matching the transparency window of an epoxy resin, light power can be converted into heat at the welding interface. This approach limits the required heating time due to a fast plasmon-induced temperature increase which locally promotes polymer crosslinking. It is shown that, by employing plasmonic nanoparticles, the curing time for a thermosetting epoxy is reduced by a factor of ten. A theoretical model which combines plasmonic heating, optical absorption, curing reaction and heat transfer is built, and quantitative agreement

between measurements and calculations is obtained by fitting experimental parameters to reasonable values. This model explains the underlying physics of the whole curing process, and provides useful guidelines to optimize the system. The nanoparticles assisted laser curing approach avoids heating the whole composite structure, serving as a versatile and efficient method of bonding materials in devices, vehicles and aircraft applications.

O-4A.4 – A Full-Spectrum Stretchable Plasmonic Pixel

Michael Semmlinger,[1,4] Ming Lun Tseng,[1,4] Jian Yang,[2,4] Chao Zhang[1,4], Peter Nordlander[1,2,4], and Naomi J. Halas[1,2,3,4]

[1]*Department of Electrical and Computer Engineering*
[2]*Department of Physics and Astronomy*
[3]*Department of Chemistry*
[4]*Laboratory for Nanophotonics*
Rice University, Houston, Texas, United States

Color pixels composed of plasmonic nanostructures provide a highly promising approach for new display technologies, capable of vivid, robust coloration and incorporating the use of low-cost plasmonic materials, such as Aluminum. However, current approaches are still quite limited in dynamical tuning range; a full color tunable plasmonic pixel is an important unmet challenge. Here we report a plasmonic pixel that can be tuned continuously across the entire visible spectrum, based on integrating Al nanostructures into an elastomeric substrate. Mechanical deformation of the flexible polydimethylsiloxane (PDMS) substrate allows for simple, quick, and reproducible tuning of the nanophotonic device. The nanostructures are rectangular shaped and assembled in a two-dimensional periodic array. By exploiting the tunability in both dimensions, this unique design enables active mechanical color tuning with unprecedented monochromaticity, while keeping elastic deformation to a minimum.
Furthermore, due to the strong sensitivity of the scattering spectrum to substrate deformation, this design can also be used to actively switch on and off pixels of different periods. In this way, this design strategy has the potential to open the door for next-generation flexible photonic devices for a wide variety of visible-light applications.

O-4A.5 – Structural Analysis by Enhanced Raman Scattering

Steven M. E. Demers,[1] James R. Matthews[1], Cyna R. Shirazinejad[1], Grace A. Isakson[1] and Jason H. Hafner[1,2]

[1]*Department of Physics, Rice University, Houston, TX*
[2]*Department of Chemistry, Rice University, Houston, TX*

Gold nanostructures focus light to a molecular length scale at their surface, creating the possibility to visualize molecular structure. The high optical intensity leads to surface enhanced Raman scattering (SERS) from nearby molecules. SERS spectra contain information on molecular position and orientation relative to the surface, but are difficult to interpret quantitatively. Here we describe a ratiometric analysis method that combines SERS and unenhanced Raman spectra with theoretical calculations of the optical field and molecular polarizability. When applied to the surfactant layer on gold nanorods, the alkane chain is found to be tilted 25° to the surface normal, which matches previous reports of the layer thickness. The analysis was also applied to fluid phase phospholipid bilayers that contain tryptophan on the surface of gold nanorods. The lipid double bond was found to be oriented normal to the bilayer and 13 Å from the nitrogen atom. Tryptophan was found to sit near the glycerol headgroup region with its indole ring 43° from the bilayer normal. Current research focuses on the orientation of various lipids and the orientation of solvents (such as DMSO) within the lipid bilayer. This

method can determine specific interfacial structure under ambient conditions, with microscopic quantities of material, and without molecular labels.

Oral Session 4B: 3:30 PM – 4:45 PM

O-4B.1 – Damping of Acoustic Vibrations of Gold Nanostructures

Chongyue Yi[1], Man-Nung Su[1], Pratiksha D. Dongare[2,3], Debadi Chakraborty[5], Wei-Shun Chang[1], John E. Sader[5], Peter Nordlander[2,4,6], Naomi J. Halas[1,3,4,6], and Stephan Link[1,4,6]*

[1] Department of Chemistry, Rice University, Houston, Texas, 77005, USA
[2] Applied Physics Graduate Program, Rice University, Houston, TX 77005, USA.
[3] Department of Physics and Astronomy, Rice University, Houston, Texas, 77005, USA.
[4] Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA.
[5] School of Mathematics and Statistics, The University of Melbourne, Melbourne, Victoria, 3010, Australia.
[6] Laboratory for Nanophotonics, Rice University, Houston, Texas, 77005, USA.

We present measurements of acoustic vibrations of single gold nanostructures prepared by e-beam lithography by performing ultrafast transient extinction spectroscopy. After removing the inhomogeneous broadening effect by carrying the measurement at single-particle level, accurate determination of acoustic vibration damping time can be achieved. Although mechanical coupling between metal structures and glass substrate was observed, the acoustic energy dissipation, which is quantitatively described by Q factor, was found to be dominated by intrinsic damping channels instead of supporting substrate-induced damping mechanism. Further control on morphology of nanorods allows us to rule out the surface defect contribution on intrinsic damping. By comparing the acoustic vibration damping process in lithographic sample with chemical prepared single crystal nanorods, we concluded that the internal crystal defect due to poor crystallinity of gold nanostructure is responsible for the heavily damped acoustic vibrations. We anticipate these results on mechanical properties of lithographic metal structures provided sufficient information about the photoacoustic imaging, highly precise sensors, high-frequency resonators and ultrafast optical switching.

O-4B.2 – Unraveling the Structure-Function Relationship of Semi-Hollow Nanorods

Lauren A. McCarthy,[1] Josée R. Daniel,[2] Anjli Kumar,[1] Matthew S. Chagnot,[3] Denis Boudreau,[2] and Emilie Ringe[1,3]

[1] *Department of Chemistry, Rice University, Houston, Texas, USA*
[2] *Département de Chimie et Centre D'optique, Photonique et Laser, Université Laval, Québec City, Québec, Canada*
[3] *Department of Materials Science and Nanoengineering, Rice University, Houston, Texas, USA*

Plasmonic metal nanoparticles have far-reaching applications to the fields of catalysis, molecular sensing, medicine, and fluorescent imaging due to their enhanced interaction with light.[1] This enhancement can be tuned by particle shape, size, local environment, and material composition. The galvanic replacement reaction (GRR) provides a robust strategy for the synthesis of semi-hollow bimetallic particles, allowing efficient manipulation of particle composition.[2] In the GRR, a more noble metal (Au, Pd, Pt) replaces a less noble metal template (Ag), and a semi-hollow bimetallic structure results. Previous work has indicated that in semi-hollow AgAu nanorods, the location of the void has an impact on the localization of the electric field around the nanoparticle.[3] In this work, we build upon these results to explore the effect of void location on the resonant energy of the nanoparticle with light. Utilizing optical single particle spectroscopy and transmission electron microscopy, we have correlated void location, void size, and particle size with the spectral properties of the semi-hollow plasmonic nanoparticles. This work unravels new ways to shape plasmon energy and near-field properties in bimetallic nanostructures, with potential application to catalysis, sensing, and memory units.

O-4B.3 – Polyvalent Bacteriophages: Emerging Opportunities to Address the Growing Challenges of Antibiotic Resistant Bacteria

Pingfeng Yu, Jacques Mathieu, and Pedro J.J. Alvarez

Department of Civil and Environmental Engineering, Rice University, Houston, Texas, 77005

Bacteriophages are virus specifically infecting and replicating within bacterial hosts. The widespread and increasing occurrence of antibiotic resistant bacteria has become a global health concern and renewed interest in phage therapy. However, the efficacy of phage therapy is limited by phage narrow host range, inefficient phage delivery and develoPMent of phage-resistance. While there is strong evidence that polyvalent (broad host-range phages) are present in natural systems, the use of enrichment isolation techniques biased selects for narrow host-range phages. Sequential multi-host isolation approaches maintained the diversity of phage library and ensured that specialist phages were diluted and that the isolated generalist phages had comparable efficiency of infection to the previous hosts. The novel isolated polyvalent phages can be produced using safe hosts, and therefore may circumvent the need to utilize pathogenic or hard-to-culture hosts during production. The phage efficacy to suppress target bacteria in the biofilm is greatly improved by phage polyvalence since certain bacteria served as a physical barrier for monovalent phage diffusion, while they might enhance polyvalent phage proliferation and facilitate their propagation through the biofilm. Overall, this research developed polyvalent phage therapy to control antibiotic resistant bacteria and may serve as alternative or supplement to antibiotics.

O-4B.4 – Aluminum Nanocrystals: a sustainable substrate for quantitative SERS-based DNA detection

Shu Tian,[1] Xiao Yang,[2] Oara Neumann[3], Peter Nordlander[2,3] and Naomi J. Halas[1,2,3]

[1]*Department of Chemistry, Rice University, Houston, TX, 77005*
[2] *Department of Physics and Astronomy, Rice University, Houston, TX, 77005*
[3] *Department of Electrical and Computer Engineering, Rice University, Houston, TX, 77005*

Since its discovery in the 1970's, surface-enhanced Raman scattering (SERS) has been primarily associated with substrates composed of nanostructured noble metals. Here we investigate chemically synthesized nanocrystal aggregates of Aluminum, an inexpensive, highly abundant, and sustainable metal, as SERS substrates. Al nanocrystal aggregates are capable of substantial near-infrared SERS enhancements, similar to Au nanoparticles. The intrinsic nanoscale surface oxide of Al nanocrystals supports molecule-substrate interactions that differ dramatically from noble metal substrates. Al nanocrystal aggregates, as synthesized, are SERS substrates that enable the first label-free detection of *ss*DNA with no modification to either the *ss*DNA or the substrate surface. The preferential affinity of the *ss*DNA phosphate backbone for the Al oxide surface preserves both the spectral features and nucleic acid cross sections relative to conventional Raman spectroscopy, enabling quantitative *ss*DNA detection and analysis.

O-4B.5 – Magnon-Crystal-Field-Transition Hybridization in ErFeO₃

Xinwei Li,[1] Ning Yuan,[2] Qi Zhang,[3] Shixun Cao,[2] Zuanming Jin,[2] Wei Ren,[2] Guohong Ma,[2] Dimitry Turchinovich,[4] and Junichiro Kono[1,5,6]

[1]*Department of Electrical and Computer Engineering,*
Rice University, Houston, Texas, USA

^{2}*Department of Physics, Shanghai University, Shanghai, China*
^{3}*Argonne National Laboratories, Lemont, Illinois, USA*
^{4}*Max Plank Institute for Polymer Research, Ackermannweg, Mainz, Germany*
^{5}*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
^{6}*Department of Material Science and NanoEngineering,*
Rice University, Houston, Texas USA

Rare-earth orthoferrite compounds $RFeO_3$ (where 'R' = a rare-earth element) exhibit various temperature- and magnetic-field-driven phase transitions while they are promising for applications in ultrafast spintronic devices. It has been suggested that strong coupling between polarized R^{3+} ions and antiferromagnetically ordered Fe^{3+} spins is behind these phase transitions and controllable ultra-fast spin dynamics, but the coupling mechanism still remains unexplained despite much previous effort on both theoretical and experimental sides. Here, as opposed to using traditional static measurement techniques, we adopted a novel optical technique to tackle this problem. We used pulsed terahertz radiation, in combination with a high magnetic field and low temperature environment, to probe optical excitations in single-crystal $ErFeO_3$. We spectroscopically resolved magnetic excitation lines related to Fe^{3+} magnons and electrical excitation lines corresponding to Er^{3+} crystal field transitions (CFTs) simultaneously. With magnetic field tuning of the resonance frequencies of both types of lines, we observed clear and consistent magnon-CFT hybridization behavior, from which the Er^{3+}-Fe^{3+} coupling strength was quantitatively determined. By changing both the temperature and sample composition, we were able to tune the coupling strength at will and determine the governing physical quantity for this hybridization behavior.

GP-A Poster Session

GP-A-01   Spectroscopic Studies of Intense Deep Blue Exciplex in NPB/TPBi:PPh₃O-Based OLEDs

Ujjal Bhattacharjee,[1, 2]Chamika Hippola,[2] Dusan Danilovic,[2] Jacob W. Petrich,[2] Joseph Shinar,[2] and Ruth Shinar[2]

[1]*Supervisor: Stephan Link, Department of Chemistry, Rice University, Houston, TX, USA*
[2]*Ames Laboratory and Iowa State University, Ames, IA, USA*

We describe a spectroscopic study of an intense deep blue (430 – 440 nm) exciplex emission from NPB/TPBi:PPh₃O OLEDs which demonstrated a maximal brightness as high as 22,000 Cd/m^2. Time-resolved and steady-state PL measurements confirm the exciplex emission from NPB/TPBi:PPh₃O (5:1)/PPh₃O.   In addition to earlier study by Monkman and coworkers [Adv. Mater. **25**, 1455 (2013)], the inclusion of PPh₃O improves the OLED performance significantly. Further studies elucidates the triplet nature of the exciplex and the emission observed has been shown to be phosphorescence in contrast to the other possibility of delayed fluorescence by triplet-triplet annihilation.

Keywords: OLEDs, Time-resolved emission spectroscopy, photoluminescence, electroluminescence, PPh₃O.

GP-A-02   Metal-Semiconductor Hybrid Plasmonic-Photonic Nanostructures for High Q-Factor Selective Thermal Emitters

Chloe F. Doiron[1] and Gururaj V. Naik[2]

[1]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*

Broadband thermal radiation may be squeezed into a narrowband by using selective thermal emitters. Unlike blackbody emitters, selective thermal emitters radiate thermal photons in a narrow spectral band and are useful in many thermal applications including thermophotovoltaic energy conversion. The narrow emission bandwidth of selective emitters is accomplished by some resonant phenomenon, and often built using refractory metals because of their thermal stability. However, refractory metals, have high optical losses and limit the quality factor of the resonance or the spectral selectivity of the emitter. On the other hand, nearly lossless semiconductors provide high spectral selectivity but with very small absorption or thermal emission (Kirchhoff's law). The limitations of both these materials may be overcome by designing resonators that include both metal and semiconductor nanostructures. The high Q photonic mode excited in the semiconductor hybridizes with the high loss plasmonic mode supported by the metal thereby providing high spectral selectivity and high thermal emissivity. Here, we experimentally demonstrate a thermal emitter based on tungsten-silicon hybrid plasmonic-photonic nanoresonator achieving a narrowband selective thermal emission with a selectivity of 1:14 and peak emissivity of 0.65 while operating in the temperature range 600-1200 K. We further show that the spectral selectivity of the thermal emitter of the hybrid plasmonic-photonic resonator may be tuned by its geometry without sacrificing peak emissivity. This demonstration provides a way to relax the trade-off between peak emissivity and spectral selectivity of a thermal emitter by using hybrid plasmonic-photonic resonances.

GP-A-03   Copper-Carbon Nanotube Composites for Electrical Applications

Pavan M. V. Raja,[1] Gibran L. Esquenazi,[1] Kourtney D. Wright,[1] Cathren E. Gowenlock,[2] and Andrew R. Barron[1, 2, 3]

[1]Department of Chemistry, Rice University, Houston, Texas, USA
[2]Energy Safety Research Institute, College of Engineering, Swansea University, Swansea, Wales, UK
[3]Center for NanoHealth, Swansea University, Swansea, Wales, UK

Recent developments related to the development of copper-carbon nanotube composites for enhanced electrical conduction and current density capacity have necessitated systematic research into how such composites can be optimally prepared. Copper, the traditional material used for electrical wiring has high conductivity, but may be limited in terms of its ampacity (or the ability to carry large current densities). Metallic, or armchair singlewalled carbon nanotubes (SWCNTs), by virtue of their hollow, high-aspect ratio structure, are conducting and have the capacity to channel large amounts of electrons through their cavities through ballistic transport. A combination of both copper and nanotubes can thus potentially lead to the creation of excellent conductors with high ampacity. While this is an exciting prospect, several challenges exist in synthesizing such composites: the lack of adhesivity between copper and carbon, quality of SWCNTs, need for optimization of the various fabrication techniques, and subsequent processing of the composites into wires and cables for use in actual electrical applications, to name a few. This poster reviews progress to date in this field of research, and attempts to provide insights into possible directions for future research and development. The learning from this study can be used to optimize the manufacture of high-quality copper-nanotube constructs in particular, and superior metal-nanomaterial composites in general.

GP-A-04   Inhibition of electrolytic dissolution pathways of gold nanorods in common physiological buffers

Charlotte Flatebo,[1,2] Sean Collins,[2] Christy Landes[2,3]
[1]Applied Physics Graduate Program, Rice University, Houston, Texas, USA
[2]Department of Chemistry, Rice University, Houston, Texas, USA
[3]Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA

Modifying electrodes with metal nanocrystals can significantly increase their Faradaic efficiency and sensitivity. These enhancements are due to the increased surface-to-volume ratios, higher surface energy of certain exposed crystal facets, and the significant increase of metal-support interactions. Gold nanocrystals are surprisingly effective electrooxidation catalysts and electrochemical sensors of biological and organic molecules. In order to retain high Faradaic efficiency and sensitivity in electrochemical systems over time, it is important to study how different electrolyte conditions affect the chemistry and morphology of gold nanocrystals under applied bias. In this study, we demonstrate that the ionic composition of complex electrolyte solutions can significantly influence the morphological stability of gold nanorod (AuNR) modified indium tin oxide anodes. Hyperspectral dark field analysis of single AuNRs and correlated scanning electron microscopy shows the introduction of small concentrations of bicarbonate and phosphate ions inhibit chloride-mediated gold dissolution pathways. At high concentrations of chloride ions, both bicarbonate and phosphate ions prevents the AuNRs from dissolving until applying highly anodic potentials (>1.7 V vs Pt/PPy quasi-reference electrode). Subjecting single AuNRs to anodic bias in sodium chloride causes plasmon resonance energy red shifts in the scattering spectrum of single AuNRs corresponding to increased aspect ratios. In contrast, subjecting bicarbonate- and phosphate-buffered saline to sufficient anodic bias causes plasmon resonance energy blue shifts corresponding to decreased aspect ratios. This work demonstrates the importance of the electrolyte composition on the stability of metal nanocrystal modified electrodes for electrocatalysis and electrochemical sensing in complex physiological environments.

GP-A-05 Modelling the Dynamical Properties of the Vestibular Hair Cell Synapse

Aravind Chenrayan G.[1], Imran Quraishi[2,] Ruth Anne Eatock[3,] Robert Raphael[1]
[1]Department of Bioengineering, Rice University, Houston, Texas, USA
[2]Department of Neurology, Yale University, New Haven, Connecticut, USA
[3]Department of Neurobiology, University of Chicago, Chicago, Illinois, USA

Over the past decades much has been unraveled about the physiology and function of ion channels, pumps and transporters within the vestibular system. Calyceal synapses are a cup like structure formed by the afferent nerve around certain sensory haircells within the utricle. However, calyceal synapses are fragile and remain hard to access; this hinders the measurement of ion concentrations and potentials within them. In our work we bring together the experimentally obtained values for the open probabilities, surface density, conductance and activation times for channels such as KNCC, HCN, Sodium-Potassium ATPase, KCC and others to form a model of the vestibular hair cell synapse.

The induction of potentials in the afferent's calyx caused by release of neurotransmitters into the synaptic cleft by discrete vesicles from the haircell is termed quantal transmission. The induction of potentials by the ionic milieu, and other cellular process is termed non-quantal transmission. Our model aims to predict and account for both modes. The main benefit of such a model is the ability to see the effects of changing parameters (eg. Voltage, ion concentration, conductance change of channels via introduction of cAMPs) on the entire gamut of channels as opposed to the investigation of single channel types by gene knockout and various voltage clamp methods that are difficult to perform on the calyceal synapse. Consolidation of our current knowledge into a representative model will help foster a conclusive explanation of the mechanotransduction processes that lead to neural encoding in the vestibular system.

GP-A-06 Laser Mediated Heterogeneous Dissolution of Single Gold Nanorods

Benjamin S. Hoener,[1] Sean S.E. Collins,[1] Silke R. Kirchner,[2] Wei-Shun Chang,[1] Stephan Link,[1,3] and Christy F. Landes,[1,3]
[1]Department of Chemistry, Rice University, Houston, Texas, United States
[2]Department of Applied Physics and Materials Science, Caltech, Pasadena, California, United States
[3]Department of Electrical Engineering, Rice University, Houston, Texas, United States

Plasmonic nanoparticles have been proposed as active and selective electrocatalysts due to local heating and hot carrier generation through local surface plasmon resonance (LSPR) excitation. The electrochemical stability of gold nanoparticles based on size and crystal structure has been extensively studied in halide solutions. However, under light excitation in addition to electrochemical potential the same plasmonic effects that enhance catalytic activity may make the nanoparticles less stable and dissolve at lower electrochemical potentials. In this work we study single plasmonic gold nanorods (AuNRs) at various electrochemical potentials with and without white light laser (WLL) excitation in an aqueous chloride electrolyte solution. As electrochemical potential was increased, AuNR dissolution was tracked by changes in the LSPR scattering spectra and confirmed with correlated SEM. WLL excitation produced heterogeneous dissolution, some AuNRs dissolved at much lower potential under WLL excitation and at a greater rate. Ongoing work will test the wavelength dependence of the WLL to determine whether the laser mediated dissolution is due to local plasmonic heating, plasmonic hot-carrier generation, or local heating of the aqueous electrolyte solution by the WLL.

GP-A-07 Time-resolved spectroelectrochemical studies of nanomaterials

Anjli Kumar,[1] Eduardo Villarreal,[2] Vivian Huang,[3] Saptarshi Das,[3] and Emilie Ringe[1,2]

[1]*Chemistry, Rice University, Houston, TX, USA*
[2]*Materials Science and Nanoengineering, Rice University, Houston, TX, USA*
[3]*Engineering Sciences and Mechanics, Penn State University, PA, USA*

Nanomaterial properties are studied using a variety of techniques (e.g., electron microscopy, optical microscopy, Raman spectroscopy, etc). Spectroelectrochemical studies enable time-resolved exploration of electrochemical reactions on material surfaces. In this study, dark-field (DF) optical microscopy and reflectance spectroscopy are used to monitor material events. DF scattering provides information regarding modifications of plasmonic nanoparticles at the single-particle level. Reflectance spectral measurements enable the exploration of the corrosion of 2D materials. These studies provide real-time information regarding modulating properties of interest for nanomaterials.

GP-A-08   The Effect on Non-Flat Interfaces on System Dynamics

Iyabo G. Lawal[1], Shrinil Shah[2], Gary Hu[3], Mario G. Madrid[4], C.W. Schwingshackl[5], M.R.W. Brake[6]
[1]*Mechanical Engineering, Rice University, Houston, Texas, USA*
[2]*Arizona State University, Tempe, Arizona, USA*
[3]*Washington University in St. Louis, St. Louis, Missouri, USA*
[4]*ISAE SUPAERO, Toulouse, France*
[5]*Imperial College London, London, United Kingdom*
[6]*Mechanical Engineering, Rice University, Houston, TX, USA*

Manufactured surfaces are never completely flat due to variability in manufacturing operations, material behavior, achievable geometric tolerances and other reasons. The curvature of surfaces is a local geometric effect that affects part-to-part variability of jointed surfaces. Joints with different interface geometries behave in unpredictable ways. Among the factors that drive the uncertainty in joint performance are frictional micro and macro sliding events, surface tribology effects, residual stress from manufacturing and assembly, loss of bolt pre-load, changes in contact area and the resulting pressure field variation around the joint. The goal of this research is to identify key variables that account for the measured uncertainty in the dynamics of jointed structures, which may have local regions of conformal and non-conformal contact due to variability inherent in the manufacturing process. Using the standard benchmark system of the Brake-Reuß beam (BRB), recommendations are made for which design parameters require higher tolerances than others to minimize variability in a cost-effective manner.   Conformal beams with strong and weak curvature are studied as well as non-conformal (flat vs. curved) beams.   Experimental and numerical approaches model and validate the physical behavior of beams to understand primary causes of non-linearity in joints with different interface geometries.

GP-A-09   Engineering MultiDomain Peptides for Controlled Release and Anisotropic Applications in Bioregeneration

I-Che Li,[1] and Jeffrey D. Hartgerink[1, 2]
[1]*Chemistry Department, Rice University, Houston, Texas, USA*
[2]*Bioengineering Department, Rice University, Houston, Texas, USA*

A variety of polymeric hydrogels that mimic the native extracellular matrix have been used in tissue engineering strategies. Among all the materials, self-assembling hydrogels have shown unique physical

properties, including injectability and shear recovery, as promising candidates for biomedical applications. Due to its highly compliant criteria for sequence selection, peptide hydrogels have been widely developed for controlled small molecule release, protein delivery, and cell encapsulation. As a type of peptide hydrogel, MultiDomain Peptides (MDPs) respond to external shearing forces and have reversible self-assembly under mild conditions. In addition, their high biocompatibility make them important candidates for regenerative strategies. In our recent works, we modify the MDP sequence to achieve controlled drug release and macroscopic anisotropy.

In the first part, we design a novel "missing tooth" self-assembling material to deliver small molecules with low water solubility controllably. Our characterization demonstrates that the gels exhibit intrafibrillar encapsulation and controlled release of hydrophobic drugs. With this design, the MDP hydrogel can be used as an effective carrier of small molecules with low water solubility. In the second part, we modify the hydrophilic exterior of the MDP to achieve organized self-assembly into parallel aligned fiber bundles. With the help of shearing forces of syringe extrusion and the incorporation of the amino acid DOPA (3,4-dihydroxyphenylalanine), the self-assembled nanofibers form an anisotropic hydrogel string under modest shear stress.

GP-A-10   Imaging Stem Cells Using MRI with Next-Generation, Surfactant-Free Gadonanotubes

Sakineh E Moghaddam,[1,2] Mayra Hernandez-Rivera,[1,2] Nicholas J Zaibaq,[1] Maria da Graça Cabreira-Hansen,[2] Lon J Wilson,[1]

[1] *Department of Chemistry, Rice University, Houston, TX, USA*
[2] *Stem Cell Center, Texas Heart Institute at St. Luke's Episcopal Hospital, Houston, TX, USA*

Among the many applications for carbon nanotubes, their use in medicine has drawn special attention due to their potential for a variety of therapeutic and diagnostic applications. However, dispersibility of these nano-carriers in a biological medium is a challenge for *in-vivo* studies. They can be functionalized by either covalent or non-covalent chemistry to produce water friendly functional bioconjugates for *in-vivo* applications. In this work, we report new functionalized and high-performance Gadonanotubes (GNTs), ultra-short carbon nanotubes containing clusters of Gd^{3+} ions, MRI contrast agent (CA) materials which are highly-water-dispersible without the need of a surfactant. The new GNT materials were obtained by an *in-situ* polymerization of acrylic acid and have extremely high T_1-weighted relaxivities of 144 $(mM\ s)^{-1}$ per Gd^{3+} ion at 1.5 T at room temperature. They have been used to safely label porcine bone-marrow-derived mesenchymal stem cells for MR imaging. The labeled cells display excellent image contrast in phantom imaging experiments, and TEM images of the labeled cells, in general, reveal presence of the CA material located within the cytoplasm with ~10^{14} Gd^{3+} ions per cell.

GP-A-11   Width dependent study of gold nanorods photoluminescence

Behnaz Ostovar [1] Yi-Yu Cai ,[2] Lawrence J. Tauzin, [2] and Stephan Link[1,2]
[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[2]*Department of Chemistry, Rice University, Houston, TX, USA*

In this research, we provide a systematic study on photoluminescence (PL) in gold nanorods (AuNRs) with different sizes. We investigated the physical origin of shortband peak in PL spectra by measuring PL spectra of different sizes of AuNR. In order to better understand the underlying mechanism for this peak, we also conducted power dependence and polarization dependence experiments. The expected outcome of this project is the better understanding of the underlying process of electronic decay pathways in plasmonic nanostructures.

GP-A-12   Water Stable Aluminum Nanocrystals

David Renard,[1] Shu Tian,[1] Christopher J. DeSantis,[2] Benjamin D. Clark,[1] and Naomi Halas[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas, United States*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, United States*

Aluminum is a promising plasmonic material capable of supporting plasmons in the ultraviolet and visible regimes. This feature, paired with its low cost, makes Al a sustainable, cheap, and powerful plasmonic metal. However, Al nanocrystals have poor stability in aqueous systems, limiting their use in many traditional plasmonic applications. Here, we present a simple method for surface functionalization of Al nanocrystals with the bio-inspired polymer, polydopamine. This treatment dramatically improves the water stability of Al nanocrystals, rendering them stable in water for over two weeks where bare Al nanocrystals degrade after only one day in water. Our polymer-functionalized Al nanocrystals have also demonstrated improved resistance to water-induced oxidation in higher temperature conditions compared to bare nanocrystals. These aqueous Al nanocrystals are well-suited to electrophoretic separation based on nanocrystal size and shape, yielding truly monodisperse populations necessary for plasmonic sensing applications. These results expand the possible implementation of Al plasmonics to a wide range of aqueous applications traditionally monopolized by Au and Ag such as bioassays and other chip-based sensors.

GP-A-13   Polymer-assisted seedless synthesis and surface modification of gold nanorods

Katherinne Requejo,[1] Anton Liopo,[1] 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*

Gold nanorods (AuNRs) are anisotropic nanoparticles that have attracted the most attention because of their unique optical properties and different size that enable applications in sensing, imaging and therapy. Although several protocols have reported the broad LSPR band tunability, few of them have focused on the synthesis of small particles in high yield and their scalability. Here, we report a novel protocol for the seedless synthesis of AuNRs in high yield with hydroquinone as weak reducing agent and poly(vinylpyrrolidone) (PVP, 10 kDa) as additive. The polymer is introduced to growth solutions during synthesis for distinct concentrations of surfactant cetyltrimethylammonium bromide (CTAB): 25, 50 or 100 mM. In addition to tuning the LSPR band from 700 to 1050 nm, the synthesis is reproducible, scalable and 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. By adding PVP, the original aspect ratio (length/width) is reduced at different extents for each surfactant concentration. In order to determine the interaction of the polymer to the nanorod surface, ATR and XPS analysis was conducted. It is suggested that PVP interacts with AuNRs through the oxygen atom of the carbonyl group. Then, surface modification with PEG-SH and MUTAB was performed for three distinct aspect ratio AuNRs without and with additive. The results indicate that the presence of PVP in MUTAB coated AuNRs increases the nanoparticle stability as compared to PEGylated or CTAB protected nanorods.

GP-A-14   Nanomachines Destroy Cancer Cells

Brian E. Troutman,[1] Robert Pal, Ph.D.[2], James M. Tour, Ph.D[3,4,5] and Richard S. Gunasekera, Ph.D.[3,6,7]
[1] *Department of Physics and Astronomy, Rice University, Houston, TX, 77005, USA*
[2]*Department of Chemistry, Durham University, Durham, UK*
[3] *Department of Chemistry, Rice University, Houston, TX, 77005, USA*
[4] *Smalley-Curl Institute and NanoCarbon Center, Rice University, Houston, TX, 77005, USA*

5Department of Materials Science and NanoEngineering, Rice University, Houston, TX, 77005, USA
6Department of BioSciences Rice University, 6100 Main St. Houston, TX 77005
7Department of Biological Sciences, University of Houston-Victoria, 3007 N. Ben Wilson Drive, Victoria, TX 77901

Prostate cancer and breast cancer are the second-highest incidence of cancer deaths among men and women in the United States, respectively. Unimolecular submersible nanomolecules consist of synthetic light-driven molecular motors (nanomachines) that utilize peptides to attach to target cells and fluorophores for their tracking. Effects of two-photon-activated nanomachines (NM) were studied in PC3 (prostate) and MCF-7 (breast) cancer cell lines. The cells were incubated with the nanomachines for 10 minutes and subsequently exposed to two-photon excitation (2PE) and imaging using propidium iodide (PI) to indicate cell death (necrosis) during imaging. Results showed that nanomachines were incorporated into cells during incubation by endocytosis and when activated by 2PE, necrosis was indicated by PI dye entering the cell cytoplasm. When compared to the control, where cells were exposed to 2PE without the nanomachines, the nanomachines in media accelerated necrosis by 50%. After incubation of nanomachines in cells, necrosis was accelerated up to 60 -75% when nanomachines entered nuclear membranes and endoplasmic reticula within the cells. It is concluded that these nanomachines opened cell membranes externally and internally causing necrosis. The use of 2PE for nanomachine activation is considered to be better for future biological in-vivo studies, due to the lack of detrimental effects caused in ultraviolet light exposure. This technology has great promise for utilization as a new cancer treatment that can destroy cancer cells without harming healthy cells and tissue.

GP-A-15   A finite element model for magnetohydrodynamic squeeze-film flows between fractal surfaces of complex geometries

Jordan R. Wagner[1] and C. Fred Higgs III[1]

1Department of Mechanical Engineering, Rice University, 6100 Main St., Houston, TX 77005, USA

(Dated: 28 July 2017)

A computational model is developed to analyze squeeze-film flows of an electrically conducting fluid in the presence of a quasi-static magnetic field; the constraining surfaces of which are fractally rough and may be of any user-defined geometry. The model is employed to analyze the performance of realistic squeeze-film bearings that appear ubiquitously in a wide range of mechanical, aerospace, and nuclear engineering systems. In particular, the potential increase in load carrying capacity attained from magnetohydrodynamic (MHD) effects and surface roughness is investigated. The MHD Reynold's equation, which contains a Lorentz body force, is derived by reduction of the coupled governing equations for electro- and fluid dynamics, namely the Maxwell and Navier-Stokes equations. Surface roughness is incorporated via a generalized Weierstrass-Mandelbrot fractal for which, when truncating the series to a finite number, yields a deterministic surface. The weak form is derived for the dimensionless MHD Reynold's equation and solved with the Galerkin finite element method (GFEM). We show that the GFEM is an advantageous solution method for problems requiring gradients from computer generated surfaces. Finally, it is shown that significant improvement in the load carrying capacity may be achieved with increased MHD effects and surface roughness.

GP-A-16   Detection of antiferromagnetic order[1] and characterizing spin-charge separation[2] with ultracold ^{6}Li in a compensated optical lattice

<u>Zhenghao Zhao</u>[1], Tsung-Lin Yang[1], Ya-Ting Chang [1], Chung-You Shih[1] and Randall G. Hulet[1]

1Department of Physics and Astronomy, Rice University, Houston, Texas, United States

We explore the physics of fermions in both 1D and 3D using ^{6}Li atoms in an optical lattice. We have detected the short-range antiferromagnetic (AFM) spin correlations in 3D Fermi-Hubbard model via Bragg scattering[3]. Our next goal is to cool the atoms to lower temperature and realize the long-range ordering. We are setting up a low noise laser and servo to reduce the heating by the lattice intensity fluctuation.

We are also studying the spin-charge separation effect in 1D system with two lattice beams. Due to the Luttinger liquid theory, fermions have different speeds of sound for spin and charge excitations. Evidence of spin-charge separation has been obtained in quantum wire tunneling experiments[4,5]. However, spin and charge dispersion have not been measured independently. Ultracold atoms provide a highly tunable system for which we may directly observe this phenomenon using Bragg spectroscopy[6].

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GP-B-01   **Multi-lobed point spread functions reveal orientation-dependent coupling of fluorescent emitters to large Ag nanowires**

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

It has been demonstrated that fluorophores close to large metallic nanowires generate non-standard point spread functions based on the position and orientation of the transition dipole. These complex point spread functions possess between one and four lobes – here we have focused our analysis on two-lobed point spread functions due to the information loss in single lobes and the relative infrequency of four-lobed point spread functions. These two-lobed point spread functions are observed in experimental data wherein stationary fluorophores are excited by surface plasmon polarition propagation along Ag nanowires, and compared to point spread functions from finite-difference time-domain simulations. This comparison allows for a general sense of preferential excitation of fluorophores based on their transition dipole orientation, providing insight into the exited surface plasmon modes supported by large Ag nanowires. In the future, this extraction of transition dipole orientation from multi-lobed point spread functions can provide further insight into heterogenous surface interactions for such applications as the development of nanocatalysts.

GP-B-02   **Anti-Stokes photoluminescence of single gold nanorods**

Yi-Yu Cai,[1] Eric Sung,[1] Lawrence J. Tauzin,[1] Behnaz Ostovar,[2] Yue Zhang,[3] Peter Nordlander[2,3] and Stephan Link[1,3]
[1]*Department of Chemistry, Rice University, Houston, TX, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[3]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*

In this research, we studied the anti-Stokes photoluminescence (PL) in gold nanorods (AuNRs). The single particle PL spectra and quantum yields are collected with different excitation wavelengths and power. We then applied the theory of Purcell effect enhanced radiative relaxation of plasmon-induced hot carriers to explain the anti-Stokes PL in AuNRs. The theory agrees with the excitation wavelength dependent and power dependent experimental results. The effect of hot carrier energy distribution and local density of photonic states on PL are addressed in this research. The results can help clarify and form a unified mechanism for both Stokes and anti-Stokes PL of AuNRs.

GP-B-03   **Understanding effects of phosphorylation on C-terminal domain of AMPA receptors using single molecule FRET**

Sudeshna Chatterjee,[1] Carina Ade,[1] Caitlin E. Nurik,[4] Drew M. Dolino,[4] Sana A Shaikh,[4] Charlotte Flatebo,[1] Taylor M Hernandez,[1] Vasanthi Jayaraman[4] Stephan Link[1,2,3] and Christy F. Landes[1,2,3]

[1]*Department of Chemistry, Rice University, Houston, Texas, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*
[3]*Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[4]*Center for Membrane Biology, Department of Biochemistry and Molecular Biology, Graduate School of Biomedical Sciences, University of Texas Health Science Center, Houston, Texas, USA*

Ionotropic glutamate receptors serve as ion channels in the neuronal membrane and are responsible for fast excitatory neurotransmission across neuronal synapses in our central nervous system. Among the four different domains of glutamate receptors, the intracellular C-terminal domain (CTD) is the most difficult one to crystallize because of its lack of secondary structural elements. Thus structural and dynamical properties of CTD is least investigated. However, being the only intracellular domain of the whole protein, CTD potentially holds a significant role in the activation-deactivation mechanism of the receptor ion channel. Phosphorylation at CTD has been known to enhance channel conductance and hypothesized to transcend channel activation-deactivation signal through structural changes. However, the exact mode of conformational changes upon phosphorylation is still not understood. Single molecule Förster resonance energy transfer (smFRET) has been used as a spectroscopic technique to probe conformational changes of a section of CTD upon phosphorylation. The results from this study are expected to provide a deeper understanding of phosphorylation induced ion channel gating mechanism and therefore contribute to the ever expanding research of targeted neuro-therapy.

GP-B-04   Nanogapped Au antennas for ultrasensitive SEIRA Spectroscopy

Liangliang Dong[1,4], Xiao Yang[2,4], Chao Zhang[3,4], Benjamin Cerjan[2,4], Linan Zhou[1,4], Yu Zhang[2,4],
Alessandro Alabastri[3,4], Peter Nordlander[2,3,4] and Naomi J. Halas[1,2,3,4]
[1]Department of Chemistry, [2]Department of Physics and Astronomy, [3]Department of Electrical and Computer Engineering,
[4]Laboratory for Nanophotonics and the Smalley-Curl Institute, Rice University, 6100 Main Street, Houston, Texas USA

Surface-enhanced infrared absorption (SEIRA) spectroscopy has outstanding potential in chemical detection as a complement to surface-enhanced Raman spectroscopy (SERS), yet it has historically lagged well behind SERS in detection sensitivity. Here we report a new ultrasensitive infrared antenna designed to bring SEIRA spectroscopy into the few-molecule detection range. Our antenna consists of a bowtie-shaped Au structure with a sub-3 nm gap, positioned to create a cavity above a reflective substrate. This 3D geometry tightly confines incident mid-infrared radiation into its ultrasmall junction, yielding a hot spot with a theoretical SEIRA enhancement factor of more than 107, which can be designed to span a range of frequencies useful for SEIRA. We quantitatively evaluated the IR detection limit of this antenna design using mixed monolayers of 4-nitrothiophenol (4-NTP) and 4-methoxythiolphenol (4-MTP). The optimized antenna structure results in the detection of ~500 molecules of 4-NTP and ~600 molecules of 4-MTP with a standard commercial FTIR spectrometer. This strategy offers a new platform for analyzing the IR vibrations of minute quantities of molecules, and lends insight into the ultimate limit of single-molecule SEIRA detection.

GP-B-05   Engineering a 3D migration model of lung adenocarcinoma tumor cells in response to cancer associated fibroblasts

Sydney M. Gibson,[1] and Mary E. Dickinson[1,2]
[1]Department of Bioengineering, Rice University Houston, TX, USA
[2]Department of Molecular Physiology and Biophysics, Baylor College of Medicine, Houston, TX, USA

Lung adenocarcinoma cells modulate their migration and metastasis in response to cancer associated fibroblasts (CAFs). Previous research suggests that CAFs support tumor's invasive behavior by altering the stromal matrix structure and secreting pro-tumorigenic factors. However, how CAFs affect lung adenocarcinoma tumor cell migration and invasiveness is still poorly understood, and these complex behaviors are difficult to observe in real time. I have developed an *in vitro* model that allows easy visualization and tracking of tumor and CAF cell interactions in 3D. Tumor spheroids made of mouse lung adenocarcinoma tumor cells (344SQs) are embedded in collagen hydrogels to replicate the 3D tumor microenvironment. Spheroids are embedded with or without CAFs. A tungsten rod is casted in the gels adjacent to the spheroid and removed after gel polymerization

to leave a 50 μm tunnel. Over 72 hours, I am able to successfully live-image 344SQs as they collectively migrate into the tunnels and not the surrounding collagen matrix. In the presence of CAFs, 344SQs follow the CAFs in a leader-follower fashion into both the tunnels and the surrounding matrix. It was also found that CAF migration speed into the tunnels is significantly enhanced in CAF-344SQ cell spheroids compared to CAF spheroids alone. This model allows easy visualization and quantification of tumor cell migration and CAF-tumor cell behaviors in a 3D microenvironment. This model can be used to understand these complex interactions in real time, providing a better understanding of lung adenocarcinoma metastasis.

GP-B-06 Multifunctional Core-Shell Nanomatryoshkas: A Nano-complex for Cancer Therapy

Luke Henderson,[1,4] Oara Neumann,[3,4] and Naomi J. Halas[1,2,3,4]

[1]Department of Chemistry, [2]Department of Material Science and Nanoengineering, [3]Department of Electrical and Computer Engineering, [4]Laboratory for Nanophotonics, 6100 Main St., Rice University, Houston, TX 77005

Multifunctional plasmonic nanostructures have demonstrated great promise for their potential in the treatment of solid tumors; however, the crucial ability to efficiently track the uptake of these particles within tumors is still lacking. We have addressed this challenge through the design and creation of theranostic core shell particles that are near-IR resonant and traceable via fluorescence and magnetic resonance imaging (MRI). This is achieved through the encapsulation of chelating agents and fluorescent dyes in an interstitial silica layer between two layers of gold known as Au nanomatryoshkas (NM). This multifunctional nanocomplex increases MRI sensitivity by concentrating $Fe(III)$ ions into the Fe-NMs and reduces the potential toxicity of $Fe(III)$ ions by preventing their release in vivo through the outer Au shell protection. A fluorescent dye was simultaneously loaded within the nanostructure and demonstrated significantly reduced photobleaching compared to the free dye, a finding that could potentially overcome a major drawback in fluorescence imaging. These novel systems could allow for not only the diagnosis and treatment of solid tumors, but also the tracking of the particles in vivo, a step essential to improve their application and safety.

GP-B-07 Circular Differential Scattering Studies of Bovine Serum Albumin Coated Nanorod Aggregates

Taylor Hernandez,[1] Kyle Smith,[1] and Qingfeng Zhang[1]

[1]Chemistry, Rice University, Houston, TX, USA

The biological fate of plasmonic nanoparticles in living systems is largely dependent on the interaction between the particle and the proteins in the system. A protein corona is formed, which alters the recognition of the particle by the cell and ultimately determines the fate of the particle. The chiral structures of proteins interact preferentially with circularly polarized light of the same handedness. When circularly polarized light is incident on a plasmonic structure that is chiral, the helical pitch of the light is reduced in size from the wavelength of the light to a scale which is more comparable with the size of tertiary and quaternary chiral structures in proteins. This size match up greatly increases the chiral signal from the chiral protein structure. When gold nanorods are placed in a low concentration solution of bovine serum albumin (BSA), the rods will aggregate. The unperturbed aggregates in solution give both the expected circular dichroism (CD) signal from BSA in the UV, and another very strong plasmon coupled signal in the visible region. In order to determine whether the aggregates themselves are chiral and contributing to the CD signal, which is likely, it is proposed that single particle circular dichroism scattering (CDS) measurements be correlated with 3D TEM tomography. In this way, the contribution to the CDS signal from the chiral plasmonic aggregate structure can be determined,

and theoretically the signal from the protein can be separated.

GP-B-08   **Imaging Protein Binding onto Gold Nanoparticle Surface: A Model System for Studying Protein Corona**

Kshipra Kapoor, [1] Christy Landes, [1,2]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, United States*
[2]*Department of Chemistry, Rice University, Houston, Texas, United States*

Nanoparticles(NPs), once introduced into a biological system, become coated with several biomolecules present in the medium. This coating is designated as the protein corona. I use single-molecule fluorescence microscopy to probe the binding of low concentration (nanomolar range) model serum protein (i.e. bovine serum albumin (BSA)) on gold NP(Au) surfaces. Previous work by the Landes group showed that, in low concentrations the proteins irreversibly attach and unfold on the NP surface resulting in irreversible aggregation. To explore the extent of unfolding of the proteins, I concentrated on the use of Au nanowires(NWs) because of their higher aspect ratio, which leads to binding of multiple BSA molecules onto a single wire's surface. Single molecule fluorescence microscopy is utilized as a spectroscopic tool to monitor the interaction of protein molecules with the NWs in real time. The single molecule data confirms multiple BSA molecules were adsorbed onto the NW surface. The trend in separation suggests the most likely smallest separation of about 400nm between multiple adsorbed BSA molecules on the nanowire and these separations seem to be anomalously large and suggest that proteins unfold upon adsorption to the NW surface. My preliminary results also suggest that there is no preferential binding of protein molecules at the ends or middle of the wires. This is the first step towards understanding the binding and extent of unfolding of the protein on nanoparticles in-situ. This deeper understanding of the nanoparticle-protein binding will result in significant contributions toward engineering nanoparticles for biomedical applications.

GP-B-09   **Evaluation of the host response to Multidomain Peptide Hydrogels**

Tania Lopez Silva[1] and Jeffrey D. Hartgerink[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas, USA*
[2]*Department of Bioengineering, Rice University, Houston, Texas, USA*

A current challenge for regenerative medicine and tissue engineering is the effective regeneration of vital organs into a functional and healthy state. A strategy to overcome this challenge is the use of biomaterials that provide support for *in situ* regeneration. The success of this approach depends on the properties and biocompatibility of the material, which needs to work as a scaffold for cell growth, attachment, and differentiation, be biodegradable, allow oxygen and nutrient exchange, and be accepted by the host without inducing immune and chronic inflammatory responses. The Hartgerink Lab developed the Multidomain Peptide hydrogels (MDP), which have demonstrated to be promising biomaterials for tissue engineering applications, including drug delivery, cellular encapsulation, angiogenesis, among others. An area of opportunity is the evaluation of the immune and inflammatory responses to MDP hydrogels, which are relevant parameters to determine the effectiveness of this material. In this project, we evaluated and characterized the immune and inflammatory responses to MDP hydrogels using the subcutaneous injection *in vivo* model. The characterization of the host response was achieved by histological analysis of the implanted material and the quantification and immunophenotyping of the cellular infiltrate using Fluorescence-Activated cell sorting (FACS). The studied MDP hydrogel showed to be rapidly infiltrated by immune cells, mostly granulocytes, monocytes, and macrophages. Also, blood vessels and nerves were found to be present within the implants. The outcomes of the project will

provide a better understanding of hydrogel interactions with the body, which will facilitate the translation of MDP hydrogels to clinical use.

GP-B-10 Thermal Model of Gas-nanocatalyst Colloid for Plasmon-induced Photocatalysis

Minhan Lou,[1] Linan Zhou,[2] Alessandro Alabastri,[3] Peter Nordlander,[1,3] and Naomi Halas[1,2,3]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, United States*
[2] *Department of Chemistry, Rice University, Houston, TX, United States*
[3] *Department of Physics and Astronomy, University or Rice University, Houston, TX, United States*

Plasmon-induced photocatalysis in nanoparticles can be attributed to an increased temperature or to a large hot carriers generation. To quantify the hot-carrier contribution, it is important to obtain the volume temperature distribution of the porous antenna-reactor sample filled with gases. The temperature distribution is simulated by using COMSOL Multiphysics steady-state 2D axisymmetric heat transfer model. Maxwell-Garnett's model and Wassiljewa model is employed to determine the thermal conductivity of the gas-antenna-reactor composite. During the experiments, a thermal camera captures the surface temperature distribution of the sample. We achieve good agreement between experimental data and theoretical data using different laser power, laser wavelength and reaction gases. We find the temperature contribution to be less than 1% of the total photocatalystic reaction.

GP-B-11 Design and Evaluation of Peptide Analogues Targeting Human Melanocortin 1 Receptor for Skin Cancer Prevention

Saghar Mowlazadeh Haghighi,[1] Yang Zhou,[1] Jonathan R. Sawyer,[1] Victor J Hruby,[1] and Minying Cai [1]

[1]*Department of Chemistry and Biochemistry, University of Arizona, Tucson, Arizona 85721, United States*

Melanoma is a lethal form skin cancer which causes more than 10,000 deaths in the U. S. annually. Skin pigmentation, which is regulated by the melanocortin 1 receptor (MC1R), is an effective protection against melanoma. However, the endogenous MC1R agonists and some of its analogues lack selectivity to MC1R and can have side effects through other melanocortin receptors. Even though many MC1R selective agonists were developed, the use of non-canonical amino acids raises safety concerns on the pharmacokinetics. Here we report the development of potent and selective hMC1R agonist with canonical amino acids. Using γ-MSH as a template, we developed the peptide Tyr-Val-Leu-Pro-His-Phe-Leu-Phe-Asp-Arg-Trp-Gly-NH$_2$ with at least 16-fold selectivity to hMC1R (EC$_{50}$= 4.5 nM). The serum stability was determined to be 17.5 min, which is ideal for inducing short term skin pigmentation. Key interactions between this peptide and hMC1R were identified through our molecular docking studies. Compound Tyr-Val-Leu-Pro-His-Phe-Leu-Phe-Asp-Arg-Trp-Gly-NH$_2$ is MC1R selective without any concerns on pharmacokinetics. Thus, this novel peptide is the ideal peptide ligand that fit into the niche as a skin care product for melanoma prevention.

GP-B-12 Extending the AgAu Galvanic Replacement Reaction to Non-Aqueous Media

Sarah M. Rehn,[1] Josée R. Daniel,[2] Denis Boudreau,[2] and Emilie Ringe[1,3]

[1]*Department of Chemistry, Rice University, Houston, Texas, USA*
[2]*Département de Chimie et Centre D'optique, Photonique et Laser, Université Laval, Québec City, Québec, Canada*
[3]*Department of Materials Science and Nanoengineering, Rice University, Houston, Texas, USA*

The galvanic replacement reaction (GRR) has been previously demonstrated as a valuable and resilient tool in the highly controlled synthesis of hollow and semi-hollow bimetallic nanostructures,[1] which have significant applications in fields such as catalysis, sensing, and imaging.[2] The GRR is a spontaneous redox reaction resulting in atoms of a sacrificial nanoparticle template being replaced with more noble metal ions in solution. In this case, a silver nanoparticle sacrificial template is replaced with gold (III) ions, creating semi-hollow plasmonic structures. Traditionally, the GRR has been a synthetic strategy appropriate only for aqueous environments[1] with few exceptions in organic media.[3-5] Here we discuss a new strategy for GRR in alcohols as well as organic media, investigating various reaction parameters such as temperature and the presence of reducing agents. Additionally, a synthetic method for pinhole closure in the resultant replaced nanostructures is explored, to allow for the investigation of beam-driven electrochemistry inspired by previous results on water-filled structures.[6] This work opens new avenues for effectively controlling the GRR under new conditions and paves the way for further elucidation of the novel properties of reconfigurable, semi-hollow, plasmonic structures.

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GP-A-13   Photoinduced force mapping of Au-Al heterodimer

<u>Xiao Yang</u>,[1,4] Thejaswi U. Tumkur,[3,4] Chao Zhang,[3,4] Peter Nordlander,[1,3,4] and Naomi J.Halas[1,2,3,4]

[1]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[2]*Department of Chemistry, Rice University, Houston, TX, USA*
[3]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[4]*Laboratory for Nanophotonics, Rice University, Houston, TX, USA*

Photoinduced force microscopy (PiFM) has been attracting a growing attention due to the ability to image the optical near-fields of nanoscale structures with high spatiotemporal resolution. Here we examine the feasibility of PiFM for tracking the wavelength dependence of near field, by comparing the photoinduced force mapping of Au-Al heterodimer and the corresponding monomer. We also demonstrate the difference between a gold tip and a silicon tip by showing the difference between the force spectra on an Al monomer both experimentally and theoretically. Finally, we reprove the advantage of Maxwell stress tensor method over the regular dipole approximation method by comparing their results with the corresponding experimental result. This study proves that PiFM is a promising technique in characterizing properties of nanostructures.

GP-B-14   Selective Sensing and Simultaneous Removal Chromium(VI) in Water Using Fluorescent Nanogold

<u>Yiyuan "Ben" Yin</u>[1, 2], Christian L. Coonrod[1, 2] and Kimberly N. Heck[1, 2] and Michael S. Wong[1, 2,3,4,5]

[2]*Department, University or Research Institute, City, State, Country*[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX*
[2]*Nanosystem Engineering Research Center for Nanotechnology-Enabled Water Treatment, Rice University, Houston, TX*
[3]*Department of Civil and Environmental Engineering, Rice University, Houston, TX*
[4]*Department of Chemistry, Rice University, Houston, TX*
[5]*Department of Material Science & Nanoengineering, Rice University, Houston, TX*

Fluorescent gold nanoclusters (Au NCs) are a promising material for selective chemical sensing and biomedical imaging. [1] However, low quantum yields (QY) and a limited understanding of the mechanistic origin of the fluorescence limit their practical implementation. [2] To overcome this we have sought to restrict the intramolecular motions of the surface ligands on the Au NCs, serving to increase the likelihood of photo-excitation leading to emission, known as the aggregation-induced emission (AIE) phenomenon. Through the physical mixing of glutathione-protected Au NCs, cationic polymer, multivalent anion precursors, and an outer silica nanoparticle shell [3,4] we have synthesized highly fluorescent, stable microcapsules (Au-NACs) that exhibit a QY of 29%: twice that of unencapsulated Au NCs with a five-fold enhancement in fluorescence emission intensity at 600 nm. Further, we demonstrated that chromium(VI) (Cr(VI)) ions can be detected in model drinking water through fluorescent quenching of the Au-NACs at concentrations as low as 0.05 μM (0.01 ppm) - 10× lower than the US regulation for total chromium in drinking water. As a practical example of this material, we incorporated these fluorescent NACs into filter paper and showed its possible use for rapid, at-home detection of Cr(VI) – analogous to a pH test strip.

GP-B-15   Multi-layer Nanoparticles with scattering/Absorption@1200nm

Ming Zhang,[1] Runmin Zhang,[1] and Peter Nordlander[1]

[1]Laboratory for Nanophotonics and the Department of Physics and Astronomy, Houston, TX, USA

Multiple nanoparticles with different materials and two different shapes (sphere and rod) are simulated through finite-difference time-domain method and Mie theory. The plasmon modes of different nanoparticles are plotted and the relation between peak position and particle parameters is analyzed. It is shown that by changing the parameters of the nanoparticles within experimental limit, the dipole modes with strong absorption can be tuned to 1200nm. Clear hybridization of multipole modes of metallic shell and core is also observed in rod-like nanoparticles. With strong resonance in the second near-infrared window of biological tissue, these particles provide a new insight for applications in medical imaging.

GP-B-16 Plasmon-induced Selective Carbon Dioxide Conversion on Earth-abundant Aluminum-cuprous Oxide Antenna-reactor Nanoparticles

Hangqi Zhao[1,2], Hossein Robatjazi[1,2], Dayne F. Swearer[2,3], Nathaniel J. Hogan[2,4], Linan Zhou[2,3], Alessandro Alabastri[2,4], Michael J. McClain[2,3], Peter Nordlander[1,2,4,5] and Naomi Halas[1,2,3,4,5]

[1]Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA
[2]Laboratory for Nanophotonics, Rice University, Houston, TX, USA
[3]Department of Chemistry, Rice University, Houston, TX, USA
[4]Department of Physics and Astronomy, Rice University, Houston, TX, USA
[5]Department of Material Science and Nanoengineering, Rice University, Houston, TX, USA

The rational combination of plasmonic nanoantennas with active transition metal-based catalysts, known as 'antenna-reactor' nanostructures, holds promise to expand the scope of chemical reactions possible with plasmonic photocatalysis. Here, we report earth-abundant embedded aluminum in cuprous oxide antenna-reactor heterostructures that operate more effectively and selectively for the reverse water-gas shift reaction under milder illumination than in conventional thermal conditions. Through rigorous comparison of the spatial temperature profile, optical absorption, and integrated electric field enhancement of the catalyst, we have been able to distinguish between competing photothermal and hot-carrier driven mechanistic pathways. The antenna-reactor geometry efficiently harnesses the plasmon resonance of aluminum to supply energetic hot-carriers and increases

optical absorption in cuprous oxide for selective carbon dioxide conversion to carbon monoxide with visible light. The transition from noble metals to aluminum based antenna-reactor heterostructures in plasmonic photocatalysis provides a sustainable route to high-value chemicals and reaffirms the practical potential of plasmon-mediated chemical transformations.

GP-ALUM Elucidating the Fluid-Particle Interaction in Binder Jet Additive Manufacturing

Joshua J. Wagner,[1] Christian R. Renovato,[1] and C. Fred Higgs III[2]
[1]*Department of Mechanical Engineering, Rice University, Houston, Texas, USA*

In binder jet additive manufacturing (AM), strongly coupled fluid-particle interaction is a primary factor governing the final quality of a 3D printed part; thus, better understanding of this complex physics will allow for the optimization and advancement of binder jet technology. Fundamentally, binder jet AM is comprised of many repetitive cycles, in which each cycle is made up of two key stages: 1) spreading of a powder material into a thin layer over a substrate, and 2) selectively joining particles by means of a fluid binder. Each cycle produces a solid cross section of the desired part in accordance to a CAD model by binding powder particles to one another to form solid points, lines, curves, and surfaces. At the end of each cycle, the build platform drops slightly and a new cross section is built on top of the preceding one forming a complete part layer-by-layer. The fluid is delivered to the powder layer in small droplets due to liquid jet breakup – the binder jet is administered from a printhead that is precisely controlled by computer software. At the instant a single droplet impinges the powder layer, a wealth of complex physics ensues. This work seeks to elucidate the predominant physics governing the fluid-particle interaction in binder jet additive manufacturing. This is a necessary precursor step in future and ongoing computational and experimental studies that will provide predictive capability of the process.

GP-STAFF Observations on interactions between seeds and nanomaterials

Seung Mook Lee[1], Pavan M. V. Raja[2], Gibran L. Esquanazi[2], and Andrew R. Barron[2, 3, 4]

[1]*Memorial High School, Houston, TX, USA*
[2]*Deptartment of Chemistry, Rice University, Houston, TX, USA*
[3]*Deptartment of Materials Science and Nanoengineering, Rice University, Houston, TX USA*
[4]*Energy Safety Research Institute; College of Engineering; Center for NanoHealth, Swansea University, Swansea, UK*

Prior studies have addressed concerns pertaining to the potential impact of nanomaterials on human/animal health and the environment. However, the question of how these modern materials can affect plant life is still being addressed, and not many reports exist in this regard, that address this question in a systematic manner. The current study focuses on the impact of pristine and purified carbon nanotubes, and iron oxide nanoparticles on the germination and growth of wheatgrass seeds in a hydroponic environment, from a mechanistic perspective. Parameters such as germination rate, mean germination time, and shoot growth rate, as specified by the International Seed Testing Association, in addition to a semi-quantitative composite score developed in-house, were evaluated and recorded over a two-week interaction period between the nanomaterials (with or without added solvents for better dispersion) and seeds/seedlings. Overall, the results revealed enhanced germination rates in the case of some of the nanotube scenarios, but the opposite effect was observed when purified SWNTs in association with the solvent, THF were used. The results of this study highlight the importance of understanding the effect of nanomaterials on the environment, especially in conjunction with adsorbed organic species, which is typically the case in a stochastic, natural interaction setting.

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