



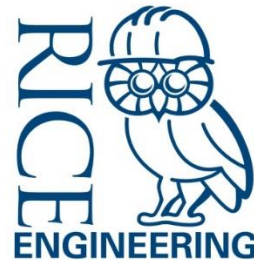
**RICE | SCI**  
**SMALLEY-CURL INSTITUTE**

## **Colloquium IV, August 10, 2018**

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Event Catered by:



# Presentation Schedule

8:00 – 8:45 AM	<b>Breakfast, Sign-in and Registration</b> (Martel Hall)	
8:45 – 9:00 AM	<b>Welcome Remarks</b> (McMurtry Auditorium) – Dr. Alberto Pimpinelli, Executive Director, Smalley-Curl Institute, and Organizing Committee Chair	
<b>Oral Session 1 (McMurtry Auditorium)</b>		
<b>Session Chair: Henry Yu</b>		
9:00 - 9:15 AM	<i>O-1.1</i> – <u>Alexander Al-Zubeidi</u> , “Photo-Electrodissolution of Single Plasmonic Nanoparticles” (co-authors B.S. Hoener, S.S.E. Collins, W. Wang, S.R. Kirchner, S.A.H. Jebeli, A. Joplin, W. Chang, S. Link, and C.F. Landes)	3
9:15 – 9:30 AM	<i>O-1.2</i> — <u>Morgan Barnes</u> , “Flat Sheets to 3D Images and Back: Programming Shape-Shifting Elastomers into Flowers, Faces and More” (co-author R. Verduzco)	
9:30 – 9:45 AM	<i>O-1.3</i> – <u>Logan Bishop</u> , “Towards Predictive Chromatography: Monte Carlo Methods and Stochastic Theory for Single Proteins Interacting with a Stationary Phase” (co-authors N.A. Moringo and C.F. Landes)	
9:45 – 10:00 AM	<i>O-1.4</i> — <u>Melia Bonomo</u> , “Modularity and hierarchy optimize target recognition in the CRISPR-Cas immune system” (co-author M. Deem)	
10:00 – 10:15 AM	<i>O-1.5</i> – <u>Luca Bursi</u> , “Universal metric for plasmonicity of excitations at the nanoscale” (co-authors R. Zhang, K.D. Chapkin, N.J. Halas, and P. Nordlander)	
10:15 AM	<b>BREAK</b>	
<b>Oral Session 2 (McMurtry Auditorium)</b>		
<b>Session Chair: Alena Klindziuk</b>		
10:30 – 10:45 AM	<i>O-2.1</i> – <u>Yiyu Cai</u> , “Purcell effect enhanced inter-/intra-band anti-Stokes photoluminescence from hot carriers generated in gold nanorods” (co-authors E. Sung, R. Zhang, L.J. Tauzin, J. Liu, B. Ostovar, Y. Zhang, C.F. Landes, W. Chang, P. Nordlander, and S. Link)	6
10:45 – 11:00 AM	<i>O-2.2</i> – <u>Fumiya Katsutani</u> , “Magnetospectroscopy of InSe up to 30 T” (co-authors A.A. Zepeda, G.T. Noe, H. Nojiri, and J. Kono)	
11:00 – 11:15 AM	<i>O-2.3</i> – <u>Aswathy Girija</u> , “Trace Gas Sensing using Infrared Spectroscopy” (co-authors W. Ye, N.P. Sanchez, and F.K. Tittel)	
11:15 – 11:30 AM	<i>O-2.4</i> – <u>Seyyed Ali Hosseini Jebeli</u> , “Absorption Localization in Plasmonic Heterodimers” (co-authors U. Batacherjee, W. Chang, and S. Link)	
11:30 – 11:45 AM	<i>O-2.5</i> – <u>Hannah Hughes</u> , “Structural Analysis of Di4-ANEPPS in a Lipid Membrane Using Enhanced Raman Scattering” (co-authors S. Demers and J. Hafner)	
11:45 AM	<b>BREAK</b>	
<b>12:00 – 1:30 PM Lunch and Afternoon Poster Sessions (Martel Hall)</b>		
	<b>Undergraduate Students (UG)</b>	9
	<b>Nakatani RIES Fellowship Undergraduate Students (NRIES)</b>	14
	<b>NEWT/RSTEM Research Experience for Undergraduates (NREU)</b>	20
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### Oral Session 3 (McMurtry Auditorium)

#### Session Chair: Hana Jaafari

- 1:30 – 1:45 PM *O-3.1* – Charlotte Flatebo, “Electrodissolution inhibition of gold nanorods with oxoanions” (co-authors S.S.E. Collins, B.S. Hoener, Y. Cai, S. Link, C.F. Landes) 32
- 1:45 – 2:00 PM *O-3.2* – David Leach, “STINGel: A Biomaterial-Based Drug Delivery Vehicle for Enhanced Cancer Immunotherapy” (co-authors N. Dharmaraj, S.L. Piotrowski, T.L. Lopez-Silva, Y.L. Lei, A.G. Sikora, S. Young, J.D. Hartgerink)
- 2:00 – 2:15 PM *O-3.3* – Duy Luong, “Laser Induced Graphene Multifunctional Composite Surface” (co-authors K. Yang, J. Yoon and J.M. Tour)
- 2:15 – 2:30 PM *O-3.4* – Lauren McCarthy, “Observation of Trochoidal Dichroism” (co-authors K.W. Smith, A.H. Jebeli, W. Chang, S. Link)
- 2:30 – 2:45 PM *O-3.5* – Ali Mojibpour, “Photon Emission by Inelastic Tunneling in Plasmonic Junctions” (co-author P. Bharadwaj)
- 2:45 PM BREAK

### Oral Session 4 (McMurtry Auditorium)

#### Session Chair: Melia Bonomo

- 3:00 – 3:15 PM *O-4.1* – Adithya Pediredla, “Elliptic path sampling for Time-of-flight rendering” (co-authors A. Veeraraghavan and I. Gkioulekas) 35
- 3:15 – 3:30 PM *O-4.2* – Dayne Swearer, “Plasmon-Assisted Ammonia Formation via Chemical Looping” (co-authors N.R. Knowles and N.J. Halas)
- 3:30 – 3:45 PM *O-4.3* – Lauren Taylor, “Washable ECG Electrodes from Sewn High Performance Carbon Nanotube Fibers” (co-authors E.A. Bengio, O.S. Dewey, F. Vitale, S.M. Williams, J.S. Yan, and M. Pasquali)
- 3:45 – 4:00 PM *O-4.4* – Lauren Warning, “Probing interfacial bovine serum albumin unfolding with single molecule high resolution imaging with photobleaching” (co-authors R. Baiyasi, Q. Zhang, S. Chatterjee, N. Moringo, J. Tauzin, C.F. Landes, and S. Link)
- 4:00 – 4:15 PM *O-4.5* – Yibo Xu, “Compressive Hyperspectral Microscopy of Nanomaterials” (co-authors A. Giljum, E. Ringe, and K.F. Kelly)
- 4:15 PM BREAK
- 4:30 – 6:00 PM **Graduate Student and Postdoctoral Researcher Poster Sessions and Reception (Martel Hall)**
- 4:30 – 5:15 PM Graduate Student and Postdoctoral Researcher Poster Session A (GP-A) Judging 38
- 5:15 – 6:00 PM Graduate Student and Postdoctoral Researcher Poster Session B (GP-B) Judging 49
- 6:15 PM **Awards Announcement and Concluding Remarks (McMurtry Auditorium)**

### **O-1.1 - Photo-Electrodissolution of Single Plasmonic Nanoparticles**

Alexander Al-Zubeidi<sup>1</sup>, Benjamin S. Hoener<sup>1</sup>, Sean S.E. Collins<sup>1</sup>, Wenxiao Wang<sup>2</sup>, Silke R. Kirchner<sup>1</sup>, Seyyed Ali Hosseini Jebeli<sup>2</sup>, Anneli Joplin<sup>1</sup>, Wei-Shun Chang<sup>1</sup>, Stephan Link<sup>1,2</sup>, Christy F. Landes<sup>1,2</sup>

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Plasmonic metal nanoparticles have become of great interest as efficient and selective photo-catalyst and as light harvesting antennas for poorly light absorbing catalysts for processes such as carbon dioxide reduction, water splitting and alkene epoxidation. Decay pathways of the light induced surface plasmon generates a high concentration of hot charge carriers on the surface of metal nanoparticles. The use of metal nanoparticles as photo-catalysts relies on extracting these hot carriers to drive redox reactions. However, due to the inherent heterogeneity of nanoparticle size and shape, and aggregation, optical and chemical properties differ vastly between individual particles, which cannot be addressed by bulk (photo-)electrochemical studies. Here, we gain single particle information by monitoring light mediated gold nanorod electrodisolution using a hyperspectral snapshot imaging method with millisecond resolution. We observe a narrow distribution of in electrodisolution onset potentials without illumination across nanoparticles, which can be lowered by 20 mV under white light laser illumination. Moreover, we observed a ten-fold increase in dissolution rate upon illumination with a white light laser. Wavelength dependent studies revealed hot holes generated from the absorption of green photons drive the dissolution reaction at almost twice the rate as red photons, indicating that highly energetic hot electrons from interband transitions can be harvested to drive electrodisolution efficiently. Enhanced mass transport due to plasmonic heating is negligible as show by calculations. This work opens up new insights into hot hole driven photocatalysis on a single particle level, while demonstrating and the importance of single particle studies for photo-catalyst studies.

### **O-1.2 - Flat Sheets to 3D Images and Back: Programming Shape-Shifting Elastomers into Flowers, Faces and More**

Morgan Barnes,<sup>1</sup> and Rafael Verduzco<sup>1,2</sup>

<sup>1</sup>*Materials Science and NanoEngineering, Rice University, Houston, TX, USA*

<sup>2</sup>*Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*

Liquid crystal elastomers (LCEs) are soft polymeric materials capable of reversibly shape-shifting in response to a variety of stimuli including heat, UV or near-IR light, and electric or magnetic fields. As such, these materials are promising in the fields of soft robotics, micro-fluidics and biomedical devices. However, current synthesis methods prohibit the facile development of complex and arbitrary shape changes. Here we present an optimized two-step synthesis method where mechanically deforming the LCE between the first and second cure steps imprints the programmed shape into the polymer network. Upon heating and cooling the LCE transitions between the initial conformation of the first cure step and the mechanically programmed shape of the second cure step, respectively. The versatility of this method to program arbitrary shape changes in LCEs is demonstrated including a flat film that reversibly curls into a flower or morphs into a human face.

### **O-1.3 - Towards Predictive Chromatography: Monte Carlo Methods and Stochastic Theory for Single Proteins Interacting with a Stationary Phase**

Logan D.C. Bishop<sup>1</sup>, Nicholas A. Moringo<sup>1</sup>, Christy F. Landes<sup>1,2</sup>

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The purification of pharmaceutically relevant proteins, termed biologics, is a complicated enterprise lacking rigorous theory to predict the outcome of an experimental separation. Many theories have been posited to describe the separatory action of chromatography, the primary method of protein purification, but all carry empirically derived assumptions that prevent accurate prediction of the final elution profile. This gap in predictive power relegates chromatographic column optimization to costly iterative empirical testing. Specifically, current theory fails to predict rare events in the column that lower separation efficiency. Using the Stochastic Theory model of chromatography, I propose a Monte Carlo simulation framework that will identify mechanisms that lower separation efficiency on a protein-by-protein basis. Using this simulation framework in tandem with single-molecule measurements, we will evaluate two mechanisms that influence separation efficiency occurring in the column: the Bayesian (conditional) nature of adsorption and concentration dependent protein competition at the stationary phase surface. Creation of the framework to solve these problems extends beyond simple identification of skewing phenomena in the column and points towards the development of purpose specific engineered chromatographic columns.

### ***O-1.4 - Modularity and hierarchy optimize target recognition in the CRISPR-Cas immune system***

Melia E. Bonomo,<sup>1,2</sup> Michael W. Deem<sup>1,2,3</sup>

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CRISPR-Cas9 has become a ubiquitous genetic editing tool for developing cell lines, disease models, and gene therapies in a variety of biotechnology and medicine applications. While the first *in vivo* human clinical trials with CRISPR-Cas9-based treatment have recently begun, there is still more to be understood about the specificity and potential off-target activity of this tool. Here, we developed a model to study the targeting activity of the endogenous CRISPR-Cas immune system in bacteria against phage, from which the genetic editing technology was derived. We based the model on experimental observations of CRISPR-Cas utilizing two main modules to recognize phage, (1) a short DNA motif called the PAM and (2) an RNA guide that matches a 30-bp DNA sequence in the phage genome. We then considered selection for additional modularity in the RNA guide based on the energy landscape of an effective targeting reaction.

We show that higher modularity in the CRISPR-Cas system leads to highly specific targeting, whereas lower modularity leads to highly cross-reactive (i.e., off-target) targeting. The canonical CRISPR-Cas system exhibits a modularity that balances these two features, being cross-reactive enough to catch phage with escape mutations while being specific enough to avoid autoimmunity. Furthermore, hierarchy emerges in the tolerance of mismatches between the RNA guide and target DNA. These results align with previous theoretical work on the non-monotonic benefit of modularity in biological systems. Our work explains the higher DNA targeting specificity observed in recent experimental work that developed CRISPR-Cas9 systems with broadened PAM compatibility.

### ***O-1.5 - Universal metric for plasmonicity of excitations at the nanoscale***

L. Bursi,<sup>1,2</sup> Runmin Zhang,<sup>1,2</sup> Kyle D. Chapkin,<sup>2,3</sup> Naomi J. Halas,<sup>1,2,3,4</sup> and P. Nordlander<sup>1,2,3,5</sup>

A recent trend in nanoplasmonics involves shrinking the size of plasmon-supporting nanostructures down to a few nanometers, thus enabling deep subwavelength manipulation of light at molecular scales, promising for sensing, photocatalysis and new optical devices.[1]

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.

Furthermore and more generally, in larger nanostructures distinguishing between plasmons and photonic modes is cumbersome, since usually even the induced charge density as well as the electric field enhancement analysis are non-trivial to interpret.

We recently introduced a *generalized plasmonicity index* (GPI) as a new descriptor, based on rigorous theoretical derivations, that ultimately provide a universal quantitative metric for the plasmonic character (or *plasmonicity*) of optical excitations in nanostructures of any size and employing virtually any computational framework.[3]

The GPI analysis of excitation properties of neutral and anionic ultrasmall PAHs – obtained exploiting *first principles* simulations based on (TD)DFT – allows us to quantitatively identify molecular plasmons among the single-particles transitions in such molecular-sized nanostructures. On the other hand, performing the same analysis on the modes of larger hybrid nanostructures (~100-300 nm) described through Classical electrodynamics enables the direct distinction of plasmons from photonic modes.[4] The connection of the GPI of a physical system in resonant condition with the Q-factor of a corresponding harmonic oscillator model is also discussed.

[1] Lauchner *et al.*, *Nano Lett.* **15**, 6208 (2015); Stec *et al.*, *ACS Nano* **11**, 3254 (2017).

[2] S. Bernadotte, *et al.*, *J.Phys.Chem.C* **117**, 1863 (2013); Krauter *et al.*, *J. Phys. Chem. C* **119**, 24564 (2015); E. B. Guidez, *et al.*, *Nanoscale* **6**, 11512 (2014); E. Townsend, *et al.*, *J.Mater.Res.* **30**, 2389 (2015); L. Bursi, *et al.*, *ACS Photonics* **1**, 1049 (2014); L. Bursi, *et al.*, *ACS Photonics* **3**, 520 (2016).

[3] R. Zhang, L. Bursi, P. Nordlander, *et al.*, *ACS Nano* **11**, 7321 (2017).

[4] K. D. Chapkin, L. Bursi, P. Nordlander, N. J. Halas, *et al.*, *to appear in PNAS* (2018).

[5] R. Zhang, L. Bursi, P. Nordlander, *in preparation*.



### **O-2.1 - Purcell effect enhanced inter-/intraband anti-Stokes photoluminescence from hot carriers generated in gold nanorods**

Yi-Yu Cai,<sup>1</sup> Eric Sung,<sup>1</sup> Runmin Zhang,<sup>2</sup> Lawrence J. Tauzin,<sup>1</sup> Jun Liu,<sup>2</sup> Behnaz Ostovar,<sup>3</sup> Yue Zhang,<sup>2</sup> Christy F. Landes,<sup>1,3</sup> Wei-Shun Chang,<sup>1</sup> Peter Nordlander,<sup>2,3,4</sup> and Stephan Link<sup>1,3</sup>

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Photoluminescence from plasmonic nanoparticles provides valuable information about hot carriers. In this work, we studied the anti-Stokes photoluminescence from single gold nanorods with continuous wave laser excitation considering the energy distribution of hot carriers and plasmonic enhancement. The two main factors explain the anti-Stokes spectral lineshape, quantum yields, and the emission polarization. Based on the band structure of gold, interband excitation gives higher anti-Stokes emission efficiency. Most importantly, we demonstrate the extract the temperature value from the PL spectra can be attributed to hot carriers, rather than phonon or lattice temperature in previous literature. Hot carriers obtaining energy from multiple excitations before reaching equilibrium with lattice dominate the anti-Stokes PL emission.

### **O-2.2 - Magneto spectroscopy of InSe up to 30 T**

Fumiya Katsutani,<sup>1</sup> André A. Zepeda,<sup>1</sup> G. Timothy Noe,<sup>1</sup> Hiroyuki Nojiri,<sup>2</sup> and Junichiro Kono<sup>1</sup>

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Atomically thin two-dimensional (2D) systems have attracted much attention during the last decade since the successful exfoliation of monolayer graphene. Among those 2D systems, semiconducting 2D materials are attractive for their applications in new devices. At the same time, they are also an ideal platform for the study of 2D excitons (or correlated electron-hole pairs), which are expected to behave very differently from excitons in bulk semiconductors, especially in a strong perpendicular magnetic field. Here, we have studied excitons in atomically thin group-III metal monochalcogenides, i.e., InSe, InS, GaSe, and GaS. These 2D materials have not been explored as much as transition metal dichalcogenides (e.g., MoS<sub>2</sub>) but are expected to exhibit dramatic changes in band structure as the number of layers decreases; in the monolayer limit, the top of the valence band is predicted to have the shape of a Mexican hat. We developed a unique experimental setup to perform circular-polarization-dependent magnetoabsorption spectroscopy measurements in pulsed high magnetic fields up to 30 T. The observed excitonic peak for InSe around 1.32 eV shifted with increasing magnetic field. When the magnetic energy is small compared with the exciton binding energy, the peak energy is expressed as  $E(B) = E(B = 0) \pm 1/2g_{\text{eff}}\mu_B B + \sigma B^2$ , where  $\sigma$  is the diamagnetic shift constant and  $g_{\text{eff}}$  is the effective g-factor. From our results, we determined  $\sigma = 4.08 \times 10^{-3} \text{ meV/T}^{-2}$  and  $g_{\text{eff}} = 2.12$ .

### **O-2.3 - Trace Gas Sensing using Infrared Spectroscopy**

Aswathy V. Girija,<sup>1</sup> Weilin Ye,<sup>1</sup> Nancy P. Sanchez<sup>2</sup>, and Frank K. Tittel<sup>1</sup>

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The development of ultra-sensitive optical sensors for real-time sensing and monitoring of greenhouse gases such as methane (CH<sub>4</sub>) and ethane (C<sub>2</sub>H<sub>6</sub>) in the atmosphere is of great importance in environmental monitoring, atmospheric chemistry and for use in the petrochemical industry. Recent advances of interband cascade lasers (ICL) have played a significant role in the development of compact sensors with high sensitivity and low power consumption. Techniques based on laser absorption spectroscopy for trace gas sensing are advantageous compared to other techniques, as they offer high gas specificity and sensitivity, provide fast response times (<1 s), and permit real-time in-situ measurements. Here, we report the spectroscopic detection and real-time monitoring of CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> based on the tunable diode laser absorption spectroscopy (TDLAS) technique. A mid-infrared ICL-based sensor system for the simultaneous detection of trace concentration levels of CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub> was demonstrated. Thermal effects of the TDLAS based sensor system was studied over a wide atmospheric temperature range and detection sensitivities of 17.4 ppbv for CH<sub>4</sub> and 2.4 ppbv for C<sub>2</sub>H<sub>6</sub> were obtained from an Allan deviation analysis, which confirms the stability of the sensor system. The reported sensor architecture has merits of significantly reduced size as well as simultaneous detection of two gases without affecting the selectivity, sensitivity and reliability.

### **O-2.4 - Absorption Localization in Plasmonic Heterodimers**

Seyyed Ali Hosseini Jebeli,<sup>1</sup> Ujjal Batacherjee,<sup>2</sup> Wei-Shun Chang,<sup>2</sup> and Stephan Link<sup>2</sup>

<sup>1</sup>*ECE Department, Rice University, Houston, TX, USA*

<sup>2</sup>*Department of Chemistry, Rice University, Houston, TX, USA*

Plasmonic structures are used in many applications like water desalination, thermos-photoavoltaic cell and photothermal therapy because of their strong absorption of light in visible and infrared region. While plasmonic structures are good absorbers in general, their absorption hotspots and consequently their temperature maps are determined by the mode that is excited. So in order to design structures with their absorption localized at a specific location, more plasmonic structures should be combined and coupled together. In this work the effect of coupling on the absorption localization is measured using photothermal contrast measurements and it has been shown that the absorption localization in coupled plasmonic structures can be controlled by changing wavelength and polarization. The effect of individual modes of the nano structures has been shown by comparing dipolar and quadropolar modes of gold nano rod dimers. This work provides the necessary information to design efficient light absorbers with localized heating in future.

### **O-2.5 - Structural Analysis of Di4-ANEPPS in a Lipid Membrane Using Enhanced Raman Scattering**

Hannah Hughes,<sup>1</sup> Steven Demers,<sup>1</sup> and Jason Hafner<sup>1,2</sup>

<sup>1</sup>*Physics and Astronomy, Rice University, Houston, TX, USA*

<sup>2</sup>*Chemistry, Rice University, Houston, TX, USA*

Here we describe the use of SABERS (Structural Analysis by Enhanced Raman Scattering) to determine the orientation of di4-ANEPPS in a model cell membrane. Gold nanostructures focus light on a molecular length scale at their surface. The high optical intensity leads to surface enhanced Raman scattering (SERS). SERS spectra contain information on molecular position and orientation but are difficult to interpret. We describe a ratiometric analysis method that combines SERS and Raman spectra with theoretical calculations of the molecular polarizability and the electric field near the nanorod surface. SERS spectra were analyzed at varying gold nanorod concentrations to reveal both the SERS and Raman contributions. The membrane probe di4-ANEPPS was inserted into the lipid bilayer and found to be oriented 58 degrees from the membrane normal

with a rotation angle of 286 degrees. This detailed knowledge of the membrane probe position in membranes can contribute to understanding the meaning of fluorescent signals from the membrane probe.

## *Undergraduate Poster Session Abstracts*

### **UG-01      Incorporation of Immune History into the $P_{\text{epitope}}$ Theory to Predict Vaccine Efficacy**

Bai Hei<sup>1</sup> and Michael W Deem<sup>1 2 3</sup>

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Seasonal influenza is a worldwide infectious disease that could be severe. Vaccination can provide protection for us, but the effectiveness will be lowered if the virus mutated from the vaccine. Our theory can predict the efficacy of vaccine with an  $r^2$  much higher than conventional method.

We already have a good result in prediction of vaccine efficacy by the  $p_{\text{epitope}}$  theory. To improve this theory, we incorporate the vaccination and infection history into it using the generalized NK model.

We assume that the probability of the mutation equals to the  $p_{\text{epitope}}$  between previous and present strains. By adding more immune history into calculation of freedom energy including interactions within a subdomain, between subdomains and of direct antibody and antigen binding, we can get the final total freedom energy ( $U_{\text{tot}}$ ) by generalized NK model.

Since the affinity constant  $K^{\text{eq}} = \exp(-bU)$ , we now have  $K^{\text{eq}}$  as the measure of the efficacy of vaccine.

We already have a better result by simply add the previous  $p_{\text{epitope}}$ s with an exponential coefficient, with an  $r^2 = 0.88$ . We are still working on combining the generalized NK model with the  $p_{\text{epitope}}$  theory and will get a better prediction.

### **UG-02      Biocompatible Small Molecule Coated Super Paramagnetic Iron Oxide Nanoparticles for Contrast-Enhanced Magnetic Resonance Imaging**

Lily Liang, Sudip Mukherjee, and Omid Veischi

*Department of Bioengineering, Rice University, Houston, Texas, United States*

Super paramagnetic iron oxide nanoparticles (SPIONs) have already been established as a successful nanoparticle contrast agent for magnetic resonance imaging (MRI) with commercial products such as Feridex or Resovist.

Recently, we have shown that a number of triazole-containing small molecules exhibit anti-fibrotic properties when coated on alginate capsules. Our aim is to screen a small library of these small molecule coated SPIONs using an initial series of constraints such as ease of synthesis, colloidal stability, hydrodynamic size, surface potential, and biocompatibility to then test magnetic resonance properties for viability as contrast agents. By isolating candidates that provide maximal magnetic resonance properties such as  $r_1$  and  $r_2$  relaxivities, and  $r_2/r_1$  relaxivity ratios compared to commercially available contrast agents, we hope to use small molecule coated SPIONs to develop a more biocompatible nanoparticle with superior magnetic properties as compared to commercial products.

### **UG-03      Incorporating glycosylation state into the $p_{\text{epitope}}$ theory**

Chi Tian,<sup>1</sup> Michael W. Deem<sup>1,2,3</sup>

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Influenza virus causes infectious disease in human and spreads on a worldwide scale. During the last century, influenza A virus has caused several pandemics with millions of deaths. To protect human from infection, a traditional precaution is vaccination. Thus, the efficacy of a vaccine is extremely important.

$P_{\text{epitope}}$  is a well-developed model for measuring antigenic distances between vaccines and viruses. It predicts vaccine efficacy based on amino acid substitutions in the dominant epitopes.

Since the emergence of influenza A virus in the human population, the virus has acquired several glycosylation sites. The glycans on the surface of the virus change the structure of the virus and shield the antigenic sites. As one of the evolution means in influenza virus, acquisition of glycosylation may help virus evade human immune system.

Here, we incorporate glycosylation into the  $p_{\text{epitope}}$  model. We predicted glycosylation by NetNGlyc, which is a commonly used program to predict N-glycosylation site occupancy based on neural net. We also included structure analysis of glycans to precisely estimate the influence of glycosylation.

We hypothesize that when glycosylation is taken into consideration the prediction by  $p_{\text{epitope}}$  will be even more accurate and reliable.

## **UG-04      Computationally-guided Evolution of Fluorescent Biosensors of Cellular Activity**

**Jin Yang<sup>1</sup>, Xiaoyu Liu<sup>2</sup>, and François St-Pierre<sup>3,4</sup>**

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<sup>2</sup>*Graduate Program in Systems, Synthetic, and Physical Biology, Rice University, Houston, TX, USA*

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Neurons compute by regulating the electrical potential (voltage) across their plasma membrane. Promising tools to quantitatively monitor voltage dynamics are fluorescent biosensors called Genetically Encoded Voltage Indicators (GEVI). However, aside from deficits in sensitivities and kinetics, many existing GEVIs have poor performance under two-photon microscopy, which limits their application for deep tissue imaging. Despite improvements of mutagenesis techniques, it remains a formidable task to do full mutagenesis on GEVIs. Structural and evolutionary approaches are still suboptimal for narrowing the search space. Therefore, the throughput of existing mutagenesis platforms has largely limited the development of better GEVIs. Here we report a high-throughput in silico pipeline using molecular dynamic (MD) simulations to guide the mutagenesis of the voltage sensing domain (VSD) of GEVIs. Conventional MD approaches are not feasible for our purpose due to the long simulation time required. We circumvent the time limitation by not running the full transition from resting to activated state but rather two independent relaxations from the homology-predicted VSD conformations of the two states. We use the distance change between S3 and S4 helices of the VSD as a proxy for the fluorescence change of GEVIs, and within the top 4 variants identified by our pipeline, we successfully predicted the best variant uncovered by experiments. We have been able to do so for three positions that we did both in silico and experimental mutagenesis on. With further calibration, we anticipate this in silico mutagenesis pipeline will be an efficient tool for accelerating the development of improved indicators.

## **UG-05      Asymmetry in Immigrant Inviability Found in Two Host-Races of a Gall Wasp Species**

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The origin of species has long been intriguing for evolutionary biologists. Studies of speciation have revealed that the formation of species can have profound ecosystem-level impacts. Due to the wide acceptance of the biological species concept, speciation research often focus on reproductive isolation. Research has shown that reproductive isolation often occurs due to divergent selection between environments, driving a process known as ecological speciation. One type of reproductive barrier crucial in ecological speciation is immigrant inviability: the reduced gene flow that results from the lower fitness of immigrants compared to that of natives. Herein, we quantify the role of immigrant inviability in reducing

gene flow between two divergently adapted populations. We use *Belonocnema treatae* (Hymenoptera: Cynipidae), a gall-forming insect that specializes on a few species of live oaks, as our study system. Through oviposition, which is an injection of venom, virus, and eggs into the tree's stem cells, the wasp causes rapid, abnormal growth of plant tissue, which serves as necessary habitat and sustenance for wasp larvae. A reciprocal transplant experiment was performed where two host-races of *B. treatae* (one adapted to the Southern Live Oak, *Quercus virginiana*, and another adapted to the Sandy Live Oak, *Q. geminata*) oviposited on native and non-native trees. Immigrant inviability was measured as the ratio of fitness of immigrants to that of natives; fitness measured as gall diameter and number of galls formed. Preliminary results suggest that *B. treatae* from *Q. virginiana* formed fewer and smaller galls on the non-native *Q. geminata* than on the native *Q. virginiana*, whereas *B. treatae* from *Q. geminata* formed fewer but larger galls on the non-native *Q. virginiana* than on the native *Q. geminata*. Such asymmetry in reproductive isolation may have significant impacts on gene flow and the progress of speciation, for which further research is needed.

## **UG-06      Approximating Frictional Force of Sliding Carbon Nanotubes within a Fiber**

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Carbon nanotubes (CNTs) are an incredible material. They are known for their strength, thermal conductivity, and electrical conductivity, all while being lightweight. Using a wet-solution spinning process, CNTs are formed into macroscopic fibers that retain these qualities. The frictional force between CNTs correlates to the tensile strength of these fibers due to the slippage between CNTs causing fiber breakage. The frictional force between these CNTs as the fibers are being pulled apart can be approximated using the Prandtl-Tomlinson Theory. The equation outlined by this theory relates temperature and the log of the strain rate to the breaking force of CNT fibers where the frictional force is used as a constant. The tensile strength of these fibers can be found by measuring their breaking force under tension. By varying both the temperature and the strain speed while measuring the breaking force under tension, we can isolate the frictional force constant. Understanding the frictional forces between CNTs at the microscopic level will help us understand the tensile strength of the fibers at the macroscopic level: a key component for the optimization of CNT fiber strength.

## **UG-07      Improving Membrane Capacitive Deionization Technology Using Sulfonated Pentablock Copolymer**

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Membrane capacitive deionization is a developing desalination technique that employs porous carbon electrodes and ion exchange membranes to remove salt ions by applying low electrical potential. The membranes used for standard MCDI study and application are provided commercially, and are not optimized for MCDI technology. In this work, a commercial multifunctional (hydrophilic, hydrophobic, charged, and mechanically robust) sulfonated pentablock copolymer was developed as a cathode coating to work towards an optimal membrane composition, and it was tested as a component of the MCDI system for efficiency and capacity. The sulfonated pentablock copolymer was dissolved into a solvent mixture (polar and non-polar) to obtain a sulfonated corona, leading to enhanced water uptake and ion transport. Three different polymer samples with varying sulfonation levels, specifically IECs of 1.0, 1.5, and 2.0 meq/g, were tested to analyze salt adsorption capacity (SAC) and charge efficiency (CE). SAC was 8.26, 8.84, and 11.14 mg/g respectively, and CE was 80, 82, and 84 % for 1.0, 1.5, and 2.0 IEC respectively. Water uptake and permeability tests were also

performed on free standing membranes with different IECs. The results indicated that membranes with a higher IEC have better water uptake and salt permeability, leading to higher salt removal performance.

## **UG-08 Quantifying the Effect of Polymer Films on Localized Surface Plasmon Resonance of Gold Nanoparticles with Hyperspectral Imaging**

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The novelty of metallic nanoparticles (NPs) resides in the highly-tunable localized surface plasmon resonance (LSPR) observed via its scattered light profile. The tunability of the LSPR stems from the size and shape of the plasmonic NPs as well as the dielectric properties of the local environment of the NPs. It is possible to harness the highly-tunable nature of the LSPR to provide opportunities for catalysis and energy storage applications; however, the LSPR must overlap with the system of interest to ensure efficiency of energy transfer between the metallic NP and the molecule of interest. To modify the LSPR without altering the shape or size of NPs, the layer-by-layer technique of depositing polymers on the surface of metallic NPs will alter the refractive index (related to the dielectric constant) of the environment surrounding the NPs, consequently shifting the LSPR. However, an optimum distance for energy transfer exists between metallic NPs and the catalytic agents, creating a two-variable problem. In this study, the effect of individual polymer layers on the LSPR of different shapes of metallic NPs is quantified with hyperspectral imaging techniques. These results will inform the selection of metallic NP and energy transfer systems for novel catalytic applications.

## **UG-09 Optical Spectroscopy of Atomically Thin InSe Encapsulated by Hexagonal Boron Nitride**

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Atomically thin two-dimensional (2D) materials have been explored since the first successful isolation of monolayer graphene in 2004. The advantages of 2D semiconductors, in comparison to quantum wells and superlattices with III-IV compounds, include being thinner and having the ability to engineer devices more easily. A decade of intense research on 2D semiconductors, such as transition metal dichalcogenides (WSe<sub>2</sub>, WS<sub>2</sub>, MoSe<sub>2</sub>, MoS<sub>2</sub>, etc.), revealed that their properties can differ greatly from the bulk material. These differences are governed by changes in the band structure due to quantum confinement, making them an exotic platform for experiments in fundamental physics. Here, we report the production and optical spectroscopic characterization of high-quality atomically thin films of indium selenide (InSe). InSe is attractive for its high electron mobility allowing for interesting applications in new devices and is also unique due to a peculiar ‘Mexican Hat’ band structure. We combined mechanical exfoliation with polydimethylsiloxane, oxygen/argon plasma cleaning, and a designed thin-film transfer setup to successfully encapsulate InSe in hexagonal boron nitride (hBN). We systematically investigated how the optical absorption and emission properties of InSe vary with the film thickness as well as with the substrate material (glass, free-standing, and hBN encapsulated). We found that hBN encapsulation increases the intensity of photoluminescence by 100X. We are currently investigating the optical behavior

of InSe samples with and without hBN encapsulation in high magnetic fields up to 30 T.

## **UG-10 Hybrid Biocomposite Films with Tuned Properties for Multifunctional Applications**

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Design of biodegradable, flexible films with the essence of multifunctional property plays an essential role in the area of composite science and technology. Here in this work, we report methods for the preparation of flexible, stretchable composite films by employing collagen and reduced graphene oxide (RGO). The composite material is a three-component system; the biopolymer and the quantum dots were prepared from the animal skin wastes, blending of collagen leads to formation of polymer and hydrothermal treatment forms quantum dots (Qdot). The Qdot and RGO were blended with the biopolymer in different weight proportions to form a flexible composite film. The thus formed films were found to exhibit improved thermal stability and physical properties. Importantly, the bio-derived films display bifunctionality and show significant electrically conducting, luminescent and are stretchable. This observation suggest that the bio-waste can be converted into useful high-value hybrid biocomposites for applications in light emitting diodes, bioelectronics, and environmental field. These approaches also highlight new avenues for turning industrial bio-wastes into useful multifunctional materials in scalable and inexpensive ways thereby minimizing environmental pollution and enhancing environmental sustainability.

## **UG-11 Coherent Terahertz Magnons up to 30 T**

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The optical manipulation of spins holds promise for technological development in the field of spintronics. Antiferromagnetic (AFM) materials are particularly advantageous for fast and reliable information transfer due to their high magnon frequency and robust magnetic structure against perturbing magnetic fields. In yttrium orthoferrite (YFeO<sub>3</sub>), a canted AFM material, there exist quasi-ferromagnetic (FM) and quasi-AFM magnon modes in the terahertz (THz) frequency range. The magnetic field component of an incident THz pulse will provide an instantaneous Zeeman torque to the quasi-FM magnetization vector, causing it to precess at the Larmor frequency in the THz range. Recently, it has been shown that one can coherently control the spins in YFeO<sub>3</sub> on a sub-picosecond timescale [1]. With the application of a strong magnetic field, the frequency of the modes will change. Here, we have recently used a single-shot THz detection system [2] to observe time-domain coherent oscillations due to magnon excitation in YFeO<sub>3</sub> in pulsed magnetic fields up to 30 T. We observed frequency splitting of the quasi-FM magnon mode as well as an additional mode that cannot be attributed to either the quasi-FM or quasi-AFM mode. These studies provide detailed new insights into the magnetic structure of canted AFM orthoferrites. We will also present recent data on a two-dimensional electron gas, and another rare-earth orthoferrite, TmFeO<sub>3</sub>, using the single-shot THz system in pulsed, high magnetic fields.

1. Z. Jin *et al.*, "Single-Pulse Terahertz Coherent Control of Spin Resonance in the Canted Antiferromagnet YFeO<sub>3</sub>, Mediated by Dielectric Anisotropy," *Phys. Rev. B* 87, 094422 (2013).



2. G. T. Noe *et al.*, “Single-Shot Terahertz Time-Domain Spectroscopy in Pulsed High Magnetic Fields,” *Optics Express* **24**, 30328 (2016).

## ***Nakatani RIES (NRIES) Poster Session Abstracts***

### ***NRIES-01 Comparing Classical and Quantum Finite Automata***

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Quantum computers offer the advantage of running more efficient algorithms because they are composed of qubits rather than conventional bits that are used in classical computers. This motivates the exploration of quantum algorithms and models with the expectation that they can solve many more complex problems. Here, we are exploring one of the simplest models of computation by comparing Deterministic Finite Automata and Quantum Finite Automata (Ambainis and Freivalds, 1998). This research focuses on applying quantum principles to the following problem: Consider a string  $a^i$  with  $i$  letters. We want to determine whether the string is in the language  $L$  where  $L = \{a^i \mid i \text{ is divisible by } p\}$  and  $p$  is a given prime number. If  $i$  is divisible by  $p$ , we accept the string into the language, and if not, we reject it.  $|0\rangle$  and  $|1\rangle$  qubit states serve as the accept and reject states. Classically, using the highest known prime integer, this algorithm requires a minimum of 77,232,917 bits, whereas the quantum finite automata only requires 27 qubits. Using Python’s Quantum Information Software Kit (Qiskit), I have implemented a program [1] that can determine if the length of a string is divisible by a large prime number with exponentially fewer qubits, thus further demonstrating the potential of quantum models.

[1] <https://github.com/kaitlinmgili/sharing-github/blob/master/Quantum%20Finite%20Automata%20Algorithm%20-2.ipynb>

### ***NRIES-02 A Study of Novel Van der Waals Heterostructures***

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Low-dimensional structures, because of their novel quantum properties, have recently attracted much interest. In addition to conventional 2D quantum wells, which have been at the heart of research, van der Waals crystals such as graphite and transition metal dichalcogenides (TMDs) have been found to be capable of being cleaved into monolayers, thus providing an ideal platform for research of low-dimensional physics. As many characteristic electronic and optical properties have already been measured for graphene and monolayer TMDs, many researchers are beginning to refocus themselves onto new heterostructures such as graphene/hexagonal boron nitride interfaces, twisted graphene systems, and heterostructures of different TMDs. Here, we report the fabrication and optical and/or electrical measurement of new van der Waals heterostructures. By using gold-mediated mechanical exfoliation and transfer techniques, we fabricated two new van der Waals heterostructures on SiO<sub>2</sub> substrates: one, WSe<sub>2</sub> on top of phosphorous, and the other, MoS<sub>2</sub> on top of ReS<sub>2</sub>. We study the optical and electronic properties of these new interfaces, and report our findings.

## ***NRIES-03 Ultrafast Carrier Dynamics of Exfoliated Transition Metal Dichalcogenides with Optical-Pump Terahertz-Probe Microscopy***

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Atomically thin two-dimensional (2D) transition metal dichalcogenides (TMD) exhibit extraordinary physical properties similar to graphene with the distinctive feature of having an intrinsic bandgap, enabling their vast potential applications in ultrafast photonic devices and optoelectronics as semiconductors. The characterization of these materials is essential for developing such technologies and the emerging terahertz (THz) microscopy proves to be an ideal technique allowing contactless probing that reveal electrical properties of microscale structures. While the optical properties of 2D TMDs have been studied extensively, their properties with respect to near-field terahertz response are not yet as well-understood. The far-field, millimeter scale nature of standard terahertz techniques is suitable for measuring the response of bulk standard semiconductors, but a terahertz microscope further reveals the carrier dynamics of TMDs. In this study, we employ a unique, optical-pump terahertz-probe microscope to measure the response of both monolayer and bulk samples of TMD MoS<sub>2</sub> and WSe<sub>2</sub> deposited on LiNbO<sub>3</sub> crystal substrate. The thin-layer TMDs were fabricated using mechanical exfoliation, resulting in pure, high-quality single crystal samples that cannot be obtained with chemical vapor deposition methods. Using optical-pump THz-probe microscopy, we measure the decay lifetime of MoS<sub>2</sub> electron carriers with a temporal resolution of approximately five hundred femtoseconds in the 1 THz range to be 8.74 picoseconds and show the THz electric field response of these thin TMDs.

## ***NRIES-04 The Effects of Structural Phase Transition on Photocatalytic Activity***

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Commercially-available photocatalysts are generally semiconducting materials which use ultraviolet radiation to create electron-hole pair which then oxidize and reduce water with no further input energy. While solar radiation is a long-term, renewable source of ultraviolet radiation, only about 4% of the solar spectrum is in the UV-range. Many prototype photocatalysts employ visible light, which makes up more than 40% of solar radiation, but the relatively low efficiency of this class of photocatalyst compared to UV-range photocatalysts means that further investigation is necessary to optimize their performance. Crystalline perovskite materials may provide a venue for improvement in this field. At the Morphotropic Phase Boundary (MPB) composition of many such materials, there is a co-existence of distinct structural phases, which gives rise to a significant amplification of the piezoelectric response of the material. However, it is as of yet unknown whether this phenomenon extends to other properties and applications of semiconducting perovskites. In an effort to provide a foundation for the improvement of visible-light photocatalysts, particularly for water splitting reactions, the photocatalytic activity of PbZr<sub>(1-x)</sub>Ti<sub>x</sub>, or PZT was observed, with an emphasis on MPB-range compositions. Much of the past research on photocatalytics has centered on surface morphology and topographical composition of photocatalysts, but this study centers on the structural phase transition and the performance of various phases in the area of water splitting.

## ***NRIES-05 Encapsulating WS<sub>2</sub> Nanoribbons in Single-walled Carbon Nanotubes***

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Transition metal dichalcogenides (TMD) carbon nanopeapods have unique electronic and magnetic properties that result from electron interactions between the carbon nanotubes (CNTs) and encapsulated low-dimensional TMDs. The hollow space of CNTs serves as a nano-test-tube to synthesize one-dimensional TMDs as opposed to two-dimensional TMDs that can be synthesized via other conventional methods. This is important because one-dimensional TMDs, like WS<sub>2</sub> nanoribbons, have interesting properties that are different from those of the bulk material due to quantum confinement. For example, according to previous research calculations, zigzag-edged WS<sub>2</sub> nanoribbons can be magnetic or nonmagnetic metals depending on the edge passivation, while bulk WS<sub>2</sub> is a nonmagnetic semiconductor<sup>[1]</sup>. Encapsulation of WS<sub>2</sub> nanoribbons inside CNTs was successfully achieved in other studies but at low yields. This research seeks to find a method to synthesize higher yields of WS<sub>2</sub> nanoribbon peapods to further study the electronic and magnetic properties of the resulting material when the nanoribbon is encapsulated and then determine possible device applications. Additionally, because this TMD nanostructure cannot be synthesized via other methods, another goal is to extract the material from the CNT because the nanoribbon has possible applications for spintronics. In this study, transmission electron microscopy was used to analyze and compare the results of different heating temperatures and times on encapsulation yields of materials inside single-walled CNTs via sublimation. From initial inter-atomic distance measurements, it appears that WS<sub>2</sub> nanoribbons were successfully encapsulated.

[1] Z. Wang, K. Zhao, H. Li, *et. al.* J. Mater. Chem., 2011, 21, 171.

## ***NRIES-06 Optimizing the Differentiation of hiPSC Derived Hepatocyte-Like Cells via Mechanical Stimulation***

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Mastering the differentiation process from human induced pluripotent stem cells (hiPSCs) to mature hepatocytes is a crucial obstacle to overcome to advance the development of the organ-on-a-chip platform. This device will be essential for the future of pre-clinical tests for drug development as it integrates multiple cell lines onto a single device<sup>[1]</sup>. Hepatocytes are essential for drug metabolism and thus would be a great asset to study in the organ on a chip. The chemical and mechanical environments during the differentiation process have been studied for several cell lines differentiated from hiPSCs, but as for hepatocytes most of the focus has been diverted to chemical stimulants, resulting in insufficient hepatocyte maturation<sup>[2]</sup>. The aim of this project is to mimic the *in vivo* conditions of the differentiation of hepatocytes during the early embryonic stage of human development where these cells are situated adjacent to the heart<sup>[3]</sup>. The recreation of the beating of the heart as a physical stimulus should lead to differentiated hepatocyte-like cells that more closely resemble real primary hepatocytes. The hiPSCs will be cultured in a poly-dimethyl siloxane (PDMS) microfluidic device that applies strain and shear stress to the cells via pulsations of the adhering surface. After 12 consecutive days of stimulus application, the mature hepatocyte-like cells will be analyzed using qRT-PCR against real primary human hepatocytes. The data collected from this experiment will improve our understanding of the differentiation of hepatocytes from hiPSCs and it will further assist in the manipulation of this process.

[1] Kamei, K. *et al.* (2017). Integrated heart/cancer on a chip to reproduce the side effects of anti-cancer drugs in vitro. *RSC Advances*, 7(58), 36777-36786. doi:10.1039/c7ra07716e

[2] Pan, D. *et al.* (2015). The role of mechanical stimuli in the vascular differentiation of mesenchymal stem cells. *Journal of Cell Science*, 128(14), 2415-2422.

[3] Zorn, A.M., Liver development (October 31, 2008), StemBook, ed. The Stem Cell Research Community, StemBook, doi/10.3824/stembook.1.25.1.

## ***NRIES-07 Understanding Carrier Density and Electric Field Effects on Valley Dynamics in 2D Transition Metal Dichalcogenides***

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Valleytronics is an emerging field of electronics and optoelectronics that aims to store information by manipulating the valley degree of freedom. Within this field, 2D transition metal dichalcogenides (TMDCs) are attracting much attention due to their unique properties that may aid in developing valleytronic devices. Currently, a major limitation of valleytronics remains its short valley polarization lifetime, or the amount of time that information can be stored<sup>[1]</sup>. Understanding the mechanism behind valley polarization is a major step towards overcoming this hurdle. In this study, we applied an out-of-plane electric field while changing carrier density as well as isolating the effect of the out-of-plane electric field. Previous attempts at investigating valleys in TMDCs have dealt with defect engineering, creation of heterostructures between two different TMDCs, and application of an out-of-plane magnetic field<sup>[2,3]</sup>. However, the carrier density and electric field effects have yet to be extensively studied experimentally, though theory has been proposed<sup>[4,5]</sup>. For testing both carrier density and electric field effects we used a WSe<sub>2</sub> monolayer placed between hBN and graphene on gold. To isolate the electric field effect, we used another device where we completely encapsulated a WSe<sub>2</sub> monolayer with hBN on gold, using graphene again to connect the electrodes. Optical measurements were carried out at low temperatures, as it has been reported that valley polarization is more pronounced<sup>[5]</sup>. We will report on the results of this experiment and its repercussions. Our research is an important step towards laying a foundation for realizing modern valleytronic applications.

[1] J.R. Schaibley *et al.* *Nature Rev. Mat.* **1**, 16055 (2016).

[2] K.P. Loh *Nat. Nanotechnol.* **12**, 837–838 (2017).

[3] A.K. Geim *et al.* *Nature* **499**, 419–425 (2013).

[4] H. Dery and Y. Song, *Phys. Rev. B* **92**, 125431 (2015).

[5] Y. Miyauchi *et al.* *Nat. Commun.* **9**, 2598 (2018).

## ***NRIES-08 CVD Graphene Nanoribbons by Silver Nanowire Shadowmasking***

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The aim of this project is to determine if CVD graphene nanoribbons are a plausible candidate for FET (Field-effect Transistor) devices. Owing to its remarkably high mobility, a CVD graphene FET would boast better performance and energy efficiency than any conventional transistor device. However, graphene in its natural, sheet form lacks a band gap, which is a prerequisite to device applications. By fabricating graphene in nanoribbon structures, a band gap is

induced that is inversely proportional to nanoribbon width. Using photo-lithography and thin film deposition techniques, gold electrodes are built over thirty nanometer diameter silver nanowires on CVD graphene. Silver nanowires provide a shadowmask for CVD graphene from oxygen plasma etching and are subsequently removed via nitric acid treatment, leaving CVD graphene nanoribbons as confirmed by AFM and electrical transport measurements. These results may serve as the precursor to fabrication of ultra-fine, large band gap CVD graphene nanoribbons by ultra-thin nanowire shadowmasking.

## ***NRIES-09* Fabrication of Wearable Heart Monitor Using Organic Amplifier Circuit**

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An aging population has led to a high demand for easy, inexpensive access to healthcare. We demonstrate the functionality of a wearable heart monitor that can benefit this situation. While modern sensors are typically rigid and silicon-based, our device utilizes an aluminum electrode deposited on polyvinylidene fluoride (PVDF) film interfaced with a Pseudo-CMOS amplifier circuit to detect pulse signals. This yields a thin, flexible system that can be worn comfortably on an individual's wrist to monitor for heart failure, heart disease, and safe exercise. The device is interfaced with a wireless module to allow for real time transmission and processing via Bluetooth. The Pseudo-CMOS circuit permits over 10x amplification of pulse signals and minimizes effects from electronic noise. Since the organic materials are soluble, the device can be manufactured inexpensively on large areas via inkjet printing. The large amplification gain and ease of fabrication provide additional applications in the fabrication of monitoring systems, flexible displays, and other biosensors, which allows for the realization of cyber-physical systems on a large scale.

## ***NRIES-10* Scanning Hall Probe Microscopy Analysis of Critical Current Density in Superconducting Materials**

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Realistic applications for superconductors abound in the realms of electronics, mechanics, and power transport. However, superconductivity relies on the microscopic properties of a material to provide the macroscopic benefits of zero resistance and incredibly high current loads. The production of superconducting wires or tapes requires that the microscopic structures of the material are carefully controlled so that current density is maximized. While the transport current density can be easily measured through four-probe testing or other simpler means, to gain an understanding of the localized critical current density or its distribution these methods prove inadequate or impractical. It is imperative that this data is obtained so that the microscopic structures that seem to limit or improve critical current can be identified and removed or replicated. The use of Hall probe microscopy allowed for the rapid analysis of current density within several superconducting samples through the measurement of their produced magnetic fields. In addition, by inducing current within the superconducting samples, the measured current densities were the critical values at the specified magnetic field strength and temperature. The inverse problem of Biot-Savart law, converting the magnetic field data into a current distribution, has been solved with a sheet current approximation in order to calculate the critical current density distribution solely from the perpendicular component of the 2-D magnetic field emitted from the sample.

## ***NRIES-11* Terahertz Emission from Aligned Carbon Nanotubes**

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There are a variety of potential applications for terahertz (THz) radiation, including security, imaging for pharmaceuticals, and various uses in medicine.<sup>1</sup> However, THz technology is poorly developed compared to microwave, infrared, and visible technology, leaving the THz frequency range as the last frontier of the electromagnetic spectrum. Some semiconductors, such as low temperature-grown gallium arsenide (LT-GaAs), have proven to be effective emitters and detectors of THz radiation, but recent theoretical studies have shown that aligned carbon nanotubes (CNTs) could provide a higher efficiency.<sup>2,3</sup> In this study, we fabricated photoconductive antenna (PCA) switches with CNT films as base material. The CNT film we used for our emitter consisted of aligned (6,5) single-wall CNTs made using a controlled vacuum filtration method.<sup>4</sup> Our PCA switches were fabricated on top of the CNT films using standard sputtering and lift-off processes. The devices were photoexcited with laser pulses of tunable wavelength from an optical parametric oscillator system, and the THz signal was directed via parabolic mirrors to our LT-GaAs detector, which was excited by laser pulses of a different frequency. Using this setup, we measured both the THz emission and induced photocurrent through the CNT sample simultaneously. By varying the experimental conditions such as laser power, wavelength, polarization, and applied bias, we were able to investigate the THz emission properties of our devices and study the dynamics that are unique to one-dimensional systems such as CNTs.

1. M. Tonouchi, *Nature Photonics*, 2007, **1**, 97-105

2. B. Heshmat, H. Pahlevaninezhad, and T. E. Darcie, *IEEE Photonics J*, 2012, **4**, 970-985

3. B. Heshmat, H. Pahlevaninezhad, M. C. Beard, C. Papadopoulos, and T. E. Darcie, *Opt. Express*, 2011, **19**, 15077-15089

4. X. He, W. Gao, L. Xie, B. Li et al., *Nature Nanotechnology*, 2016, **11**, 633-638

## ***NRIES-12* Synthesis and Characterization of Horizontally-Aligned Nanotube Heterostructures**

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Horizontally-aligned carbon nanotubes (HACNTs) are one promising morphology of single walled carbon nanotubes (SWCNTs) because of their low-defect ratios, high conductivity, and transparency, making applications like transparent displays and FETs possible<sup>[1]</sup>. Despite these properties, CNTs are limited in their widespread use due to their sensitivity to the environment and low oxidation temperature. Therefore, finding ways to protect without adversely affecting their properties is of great research interest. Recently, the Maruyama lab has realized a SWCNT-templated method for growth of boron nitride nanotubes (BNNTs), which can not only act as a protective material for the SWCNTs due to its high oxidation temperature<sup>[2]</sup> but also influence and even enhance the mechanical, electrical, and optical properties of SWCNTs. Perfectly co-axial growth of BNNTs has been established for many nanotube morphologies. The coating mechanism of HACNTs has a direct impact on potential device applications. While an understanding is greatly desired, the coating mechanism of horizontally aligned nanotubes remains unknown. To study this coating mechanism, we grew samples of HACNTs and applied our CVD BN coating method for several hours to ensure a multiwall coating. Coating evidence was confirmed through scanning electron microscopy, atomic force microscopy, and Raman spectroscopy. Once confirmed, atomically thin cross-sections were made along the alignment direction of the BNNT-HACNT sample through mechanical and chemical methods. Transmission electron microscopy was then used to observe the coating mechanism,

and some preliminary indications of the BNNT coating method have been found. Improving understanding of these heterostructures is vital toward widespread application of SWCNT electronics.

[1] Zhang, R. et al. *Chem Soc. Rev.*, 2017, **46**, 3661-3715

[2] Chen, Y et. al. *Appl. Phys. Lett.* 2004, **84**, 2430-2432

## ***NEWT/RSTEM Undergraduate Research Experience (NREU) Poster Session Abstracts***

### ***NREU-01 Cation Exchanged Layered Double Hydroxides and their Efficacy for the Removal of Selenium Oxoanions from Water***

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Layered double hydroxides (LDH),  $[M_{1-x}Al_x(OH)_2][A_{x/y}]^y \cdot nH_2O$ , (M = Co, Zn, Mg) have shown to be promising sorbents for removing both oxoanionic forms of selenium ( $Se^{4+}$ ,  $Se^{6+}$ ). To investigate the relationship between the type of metal cations in the LDH structure and the selenium removal ability, LDHs were synthesized via precipitation with M = Zn, Co, Mg, giving a mixed occupation of M, then evaluated for their removal capacities in jar tests. The effect of heat treatment on the as-precipitated LDH was also investigated to correlate the crystallinity to the removal abilities. The as-made  $Mg_2Al$  LDH and a premade, calcined  $Mg_2Al$  LDH were used to synthesize  $CoMgAl$  and  $ZnMgAl$  LDH by cation exchange. The as-precipitated LDHs were put through a hydrothermal treatment to increase the crystallinity of the LDH. X-ray diffraction (XRD), Fourier transform-infrared spectroscopy (FT-IR), and scanning electron microscopy (SEM) imaging were used for characterization. Batch tests were investigated for the removal of selenium using the as-made and the hydrothermally treated LDH. Batch tests were run with 1 and 5 ppm  $Se^{6+}$  in DI water with a LDH dosage of 0.5 g/L on an orbital shaker for 72 hrs. Mg, Co, and Zn LDH as precipitated and after hydrothermal treatment removed ~99% of the 1 ppm Se solutions, indicating that all of the LDHs were effective at removing Se under these conditions. The results indicate that altering the cations in the layers does not significantly change the removal of selenium.

### ***NREU-02 Antimicrobial Effects of Sulfidized Silver Nanoparticles (Ag-NPs) on RO Membranes***

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There are various ways to treat wastewater for purification. One method often used to effectively remove salts, contaminants, and microorganisms such as viruses and bacteria is reverse osmosis. Reverse osmosis membranes are made of a thin-film composite that allows water to permeate through the pores of the membrane, leaving behind any contaminants. However, bacteria tend to form biofilms on the surface of the membrane, increasing hydraulic resistance, and shortening membrane life expectancy. Silver, a known biocide, is used for the *in-situ* formation of silver nanoparticles (Ag-NPs) on RO membranes because of its unique antimicrobial effects. Functionalized silver membranes showed a significant reduction of live bacteria on the surface of the membrane, reducing biofouling. However, Ag-NPs are soluble, limiting their effectiveness over a short period of time. For this project, functionalized silver membranes were treated with different concentrations of  $Na_2S$  ( $10^{-1}$ ,  $10^{-3}$ , and  $10^{-5}$ ) to form  $Ag_2S$  and slow down the release of silver while preserving the antimicrobial affect. The sulfidation process resulted in a decrease of the dissolution rate of Ag-NPs. An *E. coli*-based assay was used to quantify the antimicrobial activity of the functionalized membranes at the different sulfidation levels. As expected, our results showed a negative relationship between sulfidation and antimicrobial activity: silver-functionalized membranes treated with higher concentrations of  $Na_2S$  resulted in lower toxicity to *E. coli*.

### ***NREU-03* CNTs in 3D Printing, A New Promising Approach to Water Treatment**

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Given the fast growing of additive manufacturing (AM) methods or 3D printing techniques as a promising technology with numerous applications, our bio-inspired 3D microstructure-based will offer a novel approach in the field of water treatment. The tree-mimetic design will consist of vessel-like structures, which could draw and transport water to the upper canopy structure, which would generate heat under sunlight illumination and evaporate the water. This structure will incorporate carbon nanotube (CNT), given its strong ability to absorb photons and enhanced thermal conductivity, as the functional material to boost the solar-thermal energy absorption and transformation, and steam transportation. Therefore, a significant challenge in developing such an efficient all-in-one device is to generate a hydrophilic ink containing a reasonable concentration of CNT. To achieve this goal, two critical issues were addressed: the development of photopolymers and photo-initiators suitable for water treatment and the discovery of the proper mechanical approach to disperse CNT into the photopolymer. After testing multiple monomers with a fixed concentration of CNT and photo-initiators for photopolymerization, microscopic observations, and contact angle tests, we selected the blackest ink containing acrylic photopolymer and 0.5wt% of CNT. This groundwork offers an innovative path to the manufacturing of a 3D-printed device that will offer a sustainable solution to the issue of water shortage.

### ***NREU-04* Analysis of the effect of spacer thickness and porosity on the performance of Membrane Capacitive Deionization Desalination**

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Only about one percent of the water on Earth is available as freshwater, and the amounts of freshwater available in several regions of the world has decreased due to population growth and climate change. Desalination has been and will continue to be an important solution for this worldwide challenge. Membrane Capacitive Deionization (MCDI) is a desalination technology based on the application of voltage across capacitive electrodes combined with ion exchange membranes. This project evaluated the effects of spacer porosity and spacer thickness on the desalination performance of a MCDI device. A stack was constructed with two MDCI cells with an effective single electrode size of 20 cm x 9 cm. Aqueous processed electrodes were fabricated from powdered activated carbon (PAC) with a surface area of 2,100 m<sup>2</sup>/g. Cells were constructed with electrodes, cation (CMX) and anion (AMX) exchange membranes from ASTOM-Neosepta. A 1,500 mg/L Sodium Chloride (NaCl) solution was treated at 60 s of detention time and applied voltage of 1.2V. Spacer thickness of 0.14 mm, 0.2 mm, and 0.38 mm with spacer porosity of 0.5, 0.63, and 0.77 resulted in salt adsorption capacitance of 46 F, 38F and 15 F respectively. An 8% salt removal was recorded as the maximum removal efficacy of the three experiments.

### ***NREU-05* Regeneration of silver in the removal of bromide from drinking water**

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Bromide ion (Br<sup>-</sup>) in drinking waters can react with disinfectants (such as chlorine, ozone, etc.) to produce inorganic (bromate) and organic (bromoform) disinfection by-products (DBPs) of human health concern. Silver can be used to remove bromide from water by the formation of insoluble silver bromide ( $K_{sp} = 5.2 \times 10^{-13}$ ). Although silver has been shown to remove bromide from waters (>90%), using it as a single-use technology is costly. Therefore, we developed a process using UV light to recycle the silver used for bromide treatment. This proof of concept is innovative because no one has used UV light where photons are initiating the reduction of silver halides to form silver nanoparticles and bromide ions, with water serving as the nontoxic electron donor and without any other organic scavengers in the regeneration of silver in the removal of bromide from drinking water. First, AgNO<sub>3</sub> was added to NaBr in H<sub>2</sub>O to form AgBr, and a pale-yellow precipitate was formed. Second, the precipitates were irradiated with UV light, giving them the necessary energy to start the redox process. Finally, the reduced silver nanoparticles were reused in a new NaBr in H<sub>2</sub>O. The results obtained during the first part of the experimentation using UV light confirms qualitatively the reduction of silver by the formation of a brown precipitate. After drying out the brown precipitate, it was added back to NaBr in H<sub>2</sub>O. The color change from brown to yellow indicates full cycle regeneration of silver. Future work includes quantitatively analyzing the recycling capacity of silver.

### ***NREU-06* TiO<sub>2</sub> Hierarchical Spheres Decorated With Cyclodextrin for Augmented Photocatalytic Degradation of Organic Pollutants**

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Titania, or TiO<sub>2</sub>, has been a widely researched metal oxide photocatalyst, due to its photo and chemical stability. Our project involves using hierarchical spheres of anatase TiO<sub>2</sub> as a photocatalyst and binding carboxymethyl-β-cyclodextrin (CMCD) to enhance the degradation of chemicals such as bisphenol-S, bisphenol-A, 2-naphthol, and 2,4-dichlorophenol. TiO<sub>2</sub> hierarchical spheres were synthesized through a facile hydrothermal method. TiO<sub>2</sub> were analyzed with X-Ray diffraction (XRD) to confirm that they were in the anatase form. Scanning electron microscope (SEM) was used to verify the shape, size and structures of the particles. Fourier Transform- infrared (FTIR) analysis was done to verify the anchoring of CMCD onto TiO<sub>2</sub>'s surface. Contaminants were analyzed through High Pressure/Performance Liquid Chromatography (HPLC) instrument. We measured degradation of the contaminants after the photocatalytic reaction. Our results showed that CD anchoring significantly improved the photocatalytic degradation of each contaminant. A mixture of tested contaminants also resulted in more degradation with the CMCD-TiO<sub>2</sub> particles than with the TiO<sub>2</sub> particles alone. Degradation of BPS by CMCD-TiO<sub>2</sub> was monitored for six cycles, the results show that the performance lessens progressively. However, CMCD-TiO<sub>2</sub> remains significantly stable when degrading BPA, with no decrease in photoactivity after 300 hours of use. The promising and stable photoactivity of CMCD-TiO<sub>2</sub> makes it an inviting candidate for practical photocatalytic water treatment.

### ***NREU-07* Selective Removal of Copper (Cu<sup>2+</sup>) Ion Using a MoS<sub>4</sub>-LDH Layered CDI Electrode**

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Capacitive Deionization (CDI) has shown to be an environmentally friendly, energy and cost efficient, robust system for water desalination. In CDI, brackish water is fed through two charged porous carbon electrodes that adsorb oppositely charged ions upon applying an electrical voltage. There are many types of CDI that remove all ions in solution.

However, a CDI process that can selectively remove target ions and contaminants is desirable and would significantly reduce material and operating costs. This study focused on the development of a CDI process selective for removal of  $\text{Cu}^{2+}$  through incorporation of a layered double hydroxide (LDH) material intercalated with  $\text{MoS}_4$  by layering on a CDI carbon electrode. The layered carbon electrodes were fabricated using a poly(vinyl alcohol) (PVA)/sulfosuccinic acid (SSA)/glutaraldehyde (GA) binder for LDH and  $\text{MoS}_4$ -LDH onto PCT21K activated carbon. Field emission scanning electron microscope (FE-SEM) and Fourier-transform infrared spectroscopy (FTIR) analysis confirmed the multi-layer formation of LDH on top of a porous carbon electrode. To measure surface zeta potential, electrophoretic movement analysis showed the  $\text{MoS}_4$ -LDH to be primarily negative in a pH 3-12 range. Selective desalination performance was evaluated using an electrodialysis (ED) cell and a CDI cell. With a 10 meq, 10:1 (Na:Cu) ratio feed solution, the selective ion CDI experiments showed to have a  $\text{Cu}^{2+}/\text{Na}^{1+}$  selectivity coefficient of 3.15 for zero-voltage discharge (ZVD) and 3.27 for reverse-voltage discharge (RVD). This work shows that the selectivity for both cases is similar.

## ***NREU-08* Catalytic Thermolysis of Heavy Oil with Iron(iii) p-toluenesulfonate hexahydrate**

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With the decline of conventional oil looming, the importance of heavy oil as a viable alternative is growing. The greatest obstacle to the development of heavy oil reserves is the high viscosity and API specific gravity. In our lab we investigated the viscosity reduction and in-situ upgrading of Peace River heavy crude oil under specific catalytic thermolysis. Iron(iii) p-toluenesulfonate hexahydrate was added to the heavy crude oil and thermally treated to determine the impact of the decomposition of  $\text{Fe}(\text{pts})_3$  on the viscosity. Samples of oil were thermally treated without the addition of the catalyst to compare the results. Another sample of untreated oil was used as the control. All samples' viscosity and API specific gravity were measured using a Stabinger Viscometer. Samples were then separated into SARA (Saturates, Aromatics, Resins, Asphaltenes) fractions using vacuum filtration and liquid chromatography. Analysis of each fraction was taken using X-Ray Powder Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Inductively Coupled Plasma Mass Spectrometry (ICP-MS), and Gas Chromatography (GC) to exam the impact of the decomposition of  $\text{Fe}(\text{pts})_3$ . Sulfur content was measured using Sindie sulfur analyzer. The results will be compared with previous data of similar experiments performed by one of the authors (Xu).

## ***NREU-09* Adsorption and Desorption of Oils Through Electrostatic Interactions**

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Most adsorbents used to remove oils desorb it through squeezing, combustion, or distillation, which is not ideal for large scale applications. Electrostatic repulsion between contaminant (oils) and adsorbent could be utilized in a modified filter to allow for easy desorption of the oils, thus regenerating the adsorbent material. In this study, we used glucose, zinc oxide nanoparticles, and graphite (Glc:ZnO:graphite) in a 0.25:0.20:0.05 ratio. We will be carbonizing our mixture at 1000° C with argon (Ar) gas. Adsorption will happen through hydrophobic interactions between the oils and the carbonized adsorbent material. We will be using dodecane as our contaminating oil. Desorption will happen by the addition of electrons to the graphite, creating a net negative charge in our adsorbent and generating repulsion between adsorbent and contaminant (which is hydrophobic). We have successfully adsorbed dodecane into our carbonized material (Glc/Graphite), and desorption studies are currently being optimized.

## ***NREU-10* Development of Magnetic Hybrid Nanomaterials for Silica Removal**

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The removal of silica from groundwater remains a challenge in water treatments nowadays.<sup>1</sup> Silica is a common inorganic scalant in membrane desalination systems such as reverse osmosis (RO). Scaling declines the system's efficiency by lowering water flux and clogging exposed equipment.<sup>2,3</sup> Current strategies for scaling control rely heavily on the use of anti-scalants, which prove ineffective in preventing the formation of amorphous silica scales and require hazardous processes.<sup>4</sup> The removal of silica from feedwater through adsorption mechanisms is proposed to mitigate silica scaling and decrease the use of costly anti-scalants and additional equipment. It is well known that silica is adsorbed onto metal hydroxides<sup>4</sup> such as iron<sup>5</sup> and aluminum hydroxide<sup>6</sup>, which have both shown silica removal capabilities. Herein we present the synthesis of iron-aluminum hybrid core-shell nanoparticles which combine the high silica adsorption capacity from both metal hydroxides as well as an added magnetic functionality from the superparamagnetic Fe<sub>3</sub>O<sub>4</sub> nanoparticles. The synthesized Fe<sub>3</sub>O<sub>4</sub>@Al(OH)<sub>3</sub> nanocomposite adsorbed around 87% of silica in a 2mM solution. Residual silica concentration was measured through ICP-MS and the solid material was analyzed in terms of surface composition and particle size through SEM-EDX and DLS respectively.

## ***NREU-11* Plasmon-Assisted Photo Degradation of Urea**

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Urea decomposition is a critical process in a large variety of applications including: agriculture, nylon and plastic production, explosives, medical technologies, and energy. The decomposition process leads to the production of ammonia, which is used for fertilizer, for water purification, and for the reduction of nitrogen oxides. However, the current decomposition process faces several major drawbacks: the high temperature required for the decomposition of urea (200 °C – 400 °C), the intermediate byproducts that can affect the ammonia formation, and the catalytic conditions. In this project, we showed how solar assisted Carbon black nanoparticles (CB NP) decompose urea while significantly reducing the temperature at which the reaction occurs (80 – 100 °C) as compared to traditional methods. Experiments demonstrated light-induced urea decomposition at temperatures far below the melting point of urea (~132 °C). The amount of ammonia produced was determined using a colorimetric assay. The efficiency of the decomposition process and optimization of ammonia production can be determined from the colorimetric assay. Since our project uses an off-grid geometry that can be applied at the site of need, the energy costs, risks, and hazards associated with the transport, storage and use of ammonia can be minimized.

***RSTEM-01 Constrained Paramagnetic Colloid Chain Buckling and Chain Relaxation***

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We investigate the potential manipulability of paramagnetic colloid chain configurations through the incorporation of an orthogonal magnetic field and a constraining microchannel. Expanding on previous research focused on the contractile buckling dynamics of colloid chains, we present a method for shaping the resulting configurations into uniform microsprings. Governed by bending and magnetic forces, the colloid chain configurations are manipulable through the incorporation of an external magnetic field and acute confinement. A free channel is used to experiment with various DNA linker length and magnetic field strength combinations to optimize the paramagnetic chain flexibility and inter-particle spacing. Once the colloidal chain's properties have been optimized, we propose a systematic way to control chain buckling through the incorporation of a physical constraint in the form of a microchannel, and an energetic constraint in the form of a droplet. Its confinement within the narrow microchannel provides an increased control over this final shape, resulting in the uniform microspring configuration. Additionally, we examine the relaxation rates of multiple colloid chains of varying stiffness by tracking the behavior of each mode following the removal of a linear magnetic field. Upon analyzing the different relaxation rates, we have experimentally observed that stiffer chains relax faster than those that are more flexible. This analysis will serve in furthering our understanding of the functionality of semiflexible chains as rheological probes.

***RSTEM-02 Comparison of Site-Directed Mutagenesis and Site-Saturated Mutagenesis to Explore the Effects of Amino Acids on AAV Behavior***

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Adeno-Associated Virus (AAV) is a Food and Drug Administration approved, non-pathogenic virus that is used in gene therapy by employing a virus capsid to deliver therapeutic transgenes. An AAV vector engineered to be protease responsive, known as 453-L001, has a lock sequence that inhibits virus transduction until it is cleaved by matrix metalloproteases. The full implications of the amino-acid composition of the 453-L001 lock and its effect on virus transduction are still being explored. The purpose of this study was to compare Site-Directed Mutagenesis (SDM) and Site-Saturated Mutagenesis (SSM) in order to explore the effects of amino acids on AAV transduction. Both the SDM and the SSM used the same protocol, aside from the primer design, to yield incorporation of 20 unique amino acids in 453-L001. Upon testing, SDM yielded more successful amino acid placement in 453-L001 than SSM. For the SSM reactions, two different degenerative primers were used, and resultant plasmids were sequenced using Sanger sequencing verifying the incorporation of four unique amino acids. In the SDM reaction, a specific primer set was designed for incorporation of each of the remaining 16 amino acids. In the ongoing SDM experiment, 12 of the 16 samples have been sequenced using Sanger sequencing and resulted in six unique amino acids. SDM and SSM have the same protocol and the same experimental run time. However, SDM has produced more successful amino acid placement than SSM. Therefore, SDM is the ideal approach to take to create a library of amino acids to test AAV transduction.

***RSTEM-03 Carbon Nanotube Film as Neural Electrodes***

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Chronic, stable, high resolution neural recordings are crucial for advancements in brain computer interface research. Surface electrodes are less invasive than penetrating electrodes and therefore are favored for long-term recordings. However, traditional surface electrode arrays made from metals cannot achieve the same resolution as their penetrating counterparts. This is because metal electrodes have the same functional surface area as their geometric surface area. To overcome this limitation, we propose using carbon nanotube (CNT) film as surface electrodes. Because CNT film is a percolated network, it has a high functional-to-geometric surface area ratio resulting in low impedance, and thus, improved signal-to-noise ratio (SNR). Furthermore, these films have high flexibility, excellent biocompatibility, and tunable transparency, making them a prime candidate for neural electrodes. By varying the thickness of a CNT film, we may precisely control its transparency and impedance for different applications. Highly transparent films permit simultaneous stimulation and recording, as well as optical imaging during electrophysiology. By increasing the thickness of a film and sacrificing its transparency, we can further decrease its impedance, resulting in values comparable or superior to those of metal electrodes. This allows the reduction of electrode size for improved resolution while maintaining a high SNR. Here, we establish the relationships among film transparency, conductivity, and impedance, enabling us to choose the proper film thickness for applications with different requirements. Finally, our results give us insight into whether CNT film can reach the impedance necessary for single unit recording, which has only been once demonstrated with surface electrodes.

## ***RSTEM-04* Elucidating the Role of the Dielectric Constant on Polymer Solar Cells**

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Polymer solar cells provide many advantages over traditional silicon-based photovoltaics including ease of processing, lower manufacturing cost and the potential to create flexible/stretchable devices. Despite recent advances in improving the efficiency of these devices, their performance still remains impractical for the commercial market. The efficiency of the cell is limited by the low dielectric constant of the polymers ( $\epsilon \approx 2-4$ ) which leads to tightly bound electron-hole pairs that favor recombination over dissociation into free carriers that produce photocurrent. A dielectric constant increase would enhance exciton disassociation which would give a better power conversion efficiency. Polyoxometalates (POMs) are soluble transition metal oxide clusters that could potentially provide the high dielectric constant of metal oxides while being solution processable. Here we propose the addition of  $[\text{Ta}_6\text{O}_{19}]^{8-}$  POMs into the polymer active layer to observe the effect on the dielectric constant and overall solar cell performance.

## ***RSTEM-05* Improving the dimensional accuracy of binder jet printed parts by using a material infiltration method**

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There is a growing interest in additive manufacturing, also known as 3D printing, because it enables users to print complex and highly customized objects. Three common types of 3D printing technology are binder jet printing, selective laser melting, and electron beam melting. The binder jet process consists of spreading a powder, binding the individual particles, and sintering. The binder jet process produces porous parts that must be densified with the sintering step to increase their strength. However, during sintering the geometrical structure of the printed parts often changes because of material creep. In this work, we aim to increase the dimensional accuracy in the sintering step to make printed parts more suitable for applications demanding precise geometries. We do this using an oxide precursor. The oxide precursor decomposes at temperatures above 100°C to produce titanium dioxide (TiO<sub>2</sub>) nanoparticles. These nanoparticles diffuse at lower temperature than TiO<sub>2</sub> microparticles, reinforcing the bonds between powder. We explored two methods to infiltrate green parts with the oxide precursor. Using cylindrical samples and a thermomechanical analysis system, we show that the addition of the oxide precursor has the potential to reduce shrinkage of the final parts. We also have observed a color change during sintering which corresponds to the precursor decomposition and powder oxidation. Beam samples were

also printed to study deflection. Beams with no precursor application broke down during sintering after the binder burnout around 400-500°C. The beam with precursor application did not break down and we were able to see macroscopic deflection of the beam.

## **RSTEM-06 Carbon Nanotube Wires for High Fidelity AC Signal Transfer**

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Here, electrical wires made from carbon nanotubes (CNTs) are examined as lightweight low frequency signal transfer wires. Standard metal signal transfer wires possess significant weight and are susceptible to external interference. In addition, oxidation of exposed metal conductors results in signal quality reduction. These disadvantages make them less ideal for applications in which high mobility and reliability are required. In recent years, CNT-based wires have been presented as promising replacements for metal wiring due to several attractive properties including high electrical conductivity and atmospheric stability while being lightweight. In this work, CNT wires are tailored for low frequency alternating current (AC) transfer by the inclusion of molecular dopants. Low voltage AC signals are passed through the wires and analyzed to determine transfer fidelity. Signal attenuation through the nanotube wires is examined for generated signal frequencies between 1Hz and 60MHz. Resistance to noise and external signal interference is examined between 1Hz and 200MHz. The signal transfer quality of doped CNT wires will be compared to both non-doped controls and metal wires. Based on the findings, it will be shown that CNT wires are suitable candidates for signal transfer applications ranging from high fidelity audio cabling to dependable radio frequency signal lines at a fraction of the weight of metal wiring.

## **RSTEM-07 Dual-Protease Activated Virus for Heart Disease Applications**

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Viruses are defined by many sources as “infectious” organisms, but many are currently used in the field of genetic engineering for gene therapy. “Gene therapy is an experimental technique that uses genes to treat or prevent disease.”<sup>3</sup> If successful, this could allow for the treatment of certain diseases, by inserting a gene into a patient’s cell instead of using drugs or surgical methods. This is achieved by using viruses as the gene delivery vectors.

This project focuses on utilizing Adeno-Associated virus (AAV) for the treatment of heart failure, one of the leading causes of death in America. AAV Serotype 9 (AAV9), shown in Figure 1, is used as the basis for the vector design due to its efficient transduction behavior *in vivo*. To achieve targeted gene delivery to damaged heart cells, peptide “locks” will be introduced to the capsid of the virus. These locks block the ability of the virus to deliver its transgene to cells, but in the presence of both MMPs and Caspases, two types of proteases which are upregulated in the heart failure microenvironment, the locks are removed and the virus can deliver its therapeutic payload to the diseased cells, allowing for high specificity of delivery.

## ***SCI STAR Undergraduate Participants (SSTAR) Poster Session Abstracts***

### **SSTAR-01 Sulfur-Selenium Alloy: a novel anticorrosion coating material**

Yufei (Nancy) Cui,<sup>1</sup> Sandhya Susarla<sup>2</sup>, Maqsdud Rahman<sup>2</sup>, Samuel Castro<sup>2</sup>, and Ganguli Babu<sup>2</sup>

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Corrosion is one of the most damaging and costly occurring events on materials. Specifically, the electrochemical reaction between metals and oxidizing reagents could weaken infrastructures such as pipelines and bridges, causing safety hazards and economic loss. Numerous preventive materials have been explored to resist the corrosion on the surface of constructions. In this research, a novel anticorrosion coating material: sulfur-selenium (S-Se) alloy is reported. The surface adhesion of S-Se and SS was observed using SEM. Polarization test and electric impedance spectroscopy (EIS) were conducted to test the resistance of electrochemical corrosion behavior of S-Se coated stainless steel (SS) in salt solution. It was found that S-Se coated SS shows 60 times lower corrosion rate compared with that of bare SS, reaching a protection rate of 98.3%. Thus, S-Se can be a potential candidate as an outstanding coating for constructions and marine plants to resist electrochemical corrosion.

## **SSTAR-02 Coronary Artery Extruders**

Diego Gonzalez,<sup>1</sup> Sarah Hewes,<sup>1</sup> and Dr. Jane Grande-Allen<sup>2</sup>

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The goal of this project is develop an extruder to create a multilayer hydrogel scaffold pre-seeded with cells, which can be grown into a small diameter vascular graft. These small vascular grafts could help people with Coronary Heart Disease (CHD), especially the elderly, who do have not viable replacement arteries from their own body or those who do not wish to undergo a second procedure. CHD is the most common form of heart disease which kills about 370,000 people annually. These multilayer artificial arteries are designed to mimic the natural coaxial structure found in human arteries. We used a 3D resin printer to achieve the high resolution necessary to fabricate the coronary artery extruders. Resin 3D printers achieve high detail prints by projecting a pattern of light to solidify layers of resin in a process called stereolithography. Through the continual refinement of the extruder design, the grafts produced by the extruder achieved a similar outer diameter and wall thickness to that found within a saphenous human vein. Further refinement of the extruder design and better standardization of extrusion rate is necessary for future iterations. Such adjustments will allow more focus to be placed on graft ECM composition for similar saphenous vein mechanical properties and optimal cell growth.

## **SSTAR-03 Using Hydrogel Coatings to Extend Heart Valve Lifespans**

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Patients are outliving their bioprosthetic valve (BPV) replacements thanks to recent medical advances. BPV failures force patients to undergo additional procedures, which is costly and detrimental to patients' quality of life. There is a need to improve the lifespan of BPVs to reduce re-implantation surgeries. The leading cause for BPV failure is calcification of the valve leaflets, which happens when calcium deposits develop in the tissue. The aim of our research is to prevent this buildup by coating BPVs with PEGDAA (poly(ethylene glycol) diacrylamide) hydrogel coating. This PEGDAA coating acts as a shield and should inhibit calcium deposition thus preventing calcification. Our lab has pioneered a two-step coating process that chemically crosslinks PEGDAA to the surface of tissue. An initial reaction uses primary surface amines of tissue to attach acylate groups while glucose is also adsorbed. In the second reaction, the interaction between diffusing glucose and glucose oxidase creates free radicals that propagate the formation of hydrogel attached at the acrylated surface. Preliminary results in our research have found significant reductions in protein absorption on coated valve tissue, providing hope for prevention of valve calcification with these methods. Currently, over 300,000 surgeries are needed in the US alone to remove and replace failed BPVs. Through this research, we hope to minimize failure of BPVs and significantly reduce the need for re-implantation surgery. Furthermore, our coating process can be applied to other prosthetic devices with free amines that degrade in the body and is not limited to heart valves.

## **SSTAR-04 Whole-Brain Imaging of Brief Sleep States in *C. elegans***

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Sleep is universal across animals and is characterized by distinct behavioral traits. However, how the brain regulates sleep is not well understood. The only way to study how the entire brain works together to drive sleep is to record from every neuron in the animal during sleep-wake transitions. Therefore, we used the microscopic roundworm, *Caenorhabditis elegans*, to perform whole-brain fluorescence imaging. These 3D volumetric images captured the activity of every neuron in the worm head when animals confined to microfluidic chambers spontaneously transitioned between normal activity and brief sleep bouts. Working with chemically-paralyzed animals first, we confirmed work from other groups showing a large scale down-regulation of activity across most of the brain during sleep. We then developed a system that enabled imaging in behaving animals to directly correlate neuronal activity with behavioral output. Here as well, we showed down-regulated activity across the head ganglia during sleep. However, in both paralyzed and behaving animals, a small subset of neurons displayed significantly higher activity during sleep, suggesting their roles in controlling the sleep state. Therefore, our data show that a *C. elegans* sleep-promoting circuit can rapidly and spontaneously switch the entire brain between distinct global states. Looking more closely at the transitions from sleep to wake, we observed a rapid increase in activity for several neurons 5 to 10 seconds prior to the initiation of head movement. With computational analysis in the future, we hope to link the identity and activity of these neurons to the dynamics of sleep-wake transitions.

## **SSTAR-05 Ammonia Production through Plasmon-Mediated Solar Chemical Looping**

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The Haber-Bosch process for the synthesis of ammonia is responsible for providing the basis of nutrition for nearly half of the world's population. However, this process is unsustainable due to its extreme energy requirements and undesirable by-products, producing nearly 370 million tons of CO<sub>2</sub> annually. Here, we propose a sustainable method for the synthesis of ammonia through a light-driven chemical looping process. The chemical looping process we have designed consists of three steps: 1) Mg metal is exposed to gaseous nitrogen forming Mg<sub>3</sub>N<sub>2</sub> 2) Mg<sub>3</sub>N<sub>2</sub> is hydrolyzed with water to produce ammonia and MgO and 3) MgO is reduced with methane back to Mg metal, allowing the catalytic cycle to continue. To achieve this we utilized antenna-reactor nanoparticles, which couple the catalytic magnesium component to a plasmonic nanoantenna that concentrates the energy from light into a localized heat source. A combination of mass spectrometry and rotational spectroscopy were used to monitor the chemical looping reactions and determine the output at each stage of the cycle. We observed maximum yields of NH<sub>3</sub> approaching 30 mmol/g/hr during the hydrolysis step. Future work will include utilizing a solar reactor to drive the reaction and optimizing experimental efficiencies for the overall process.

## **SSTAR-06 Thiolated Poly(Glycolic Acid) Macromers for Osteochondral Repair**

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Cartilage tissue lacks a large supply of blood vessels, so it cannot repair itself very easily. Currently, surgery is the only option to repair articular cartilage damage, but surgery is costly and leaves behind poorly-functional scar tissue. Osteochondral tissue engineering investigates the use of hydrogels or other synthetic scaffolds for osteochondral repair as



a better alternative to produce functional tissue. By delivering biomolecules such as chondroitin sulfate, a cartilage-specific biomolecule, or the protein N-cadherin to hydrogels, it is possible to stimulate the body's natural process of chondrogenesis to produce cartilage from implanted mesenchymal stem cells. Current osteochondral tissue engineering methods use microparticles and other vehicles to deliver tissue-compatible biomolecules within synthetic hydrogels. "Click" binding can be used as a more effective method to directly conjugate biomolecules to the hydrogels. First, different reactions were performed to determine the best molar equivalents of glycolide relative to poly(ethylene glycol) for a crosslinker to create a crosslinked hydrogel system. The N-cadherin peptide was also synthesized using solid-phase peptide synthesis. Next, a full factorial study testing the optimal conditions for "click" binding of an azide-presenting biomolecules revealed that "click" binding for the chondroitin sulfate biomolecule is ideal at 24 hours reaction time, 45° C, and 1 mol eq PP-BDT. Finally, degradation studies were performed on the crosslinked hydrogels conjugated to biomolecules to help determine whether the hydrogel could degrade within a reasonable timeframe for potential future implantation.

## **SSTAR-07 Momentum Distribution Properties of Ultracold Hard-Core Anyons in One Dimension**

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Using the anyon-fermion mapping, we study the properties of the single-particle momentum distribution for two hard-core anyons in the two-body ground state of a one-dimensional harmonic trap. We show through analytic and numerical techniques that the single-particle momentum distribution decays as  $p^{-4}$  at large momentum  $p$  and that the momentum tail coefficient varies with the anyon parameter  $\kappa$  as  $\cos^2(\pi\kappa/2)$ . Additionally, using a scaling transformation, we explore the dynamics for two hard-core anyons confined in a harmonic trap with a time-dependent trap frequency. When two hard-core bosons are confined in a harmonic trap and the trap is suddenly turned off, it has been shown that the gas will expand and that its single-particle momentum distribution will be the same as that of two fermions. This phenomenon is known as dynamical fermionization. We show that the same process occurs for two hard-core anyons, and we find the time-dependence of the momentum tail coefficient.

## **SSTAR-08 Overcoming Biological Barriers in Drug Delivery: Tumor Flow & Vasculature Characterization for Improved iNPG Design**

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Currently, the major cause of poor outcome in metastasis treatment is drug delivery specificity [1, 2]. In fact, after systemic injection, drugs must overcome the natural defenses of the body, called biological barriers, in order to reach the tumor site [1, 2, 3]. An Injectable Nanoparticle Generator (iNPG) has been recently developed to sequentially overcome biological barriers, which resulted in unprecedented success in metastatic breast cancer treatment [4]. The first stage of iNPG is the silicon discoidal microparticle that accumulates in the tumor vasculature due to its size and shape [4, 5]. This preferential tumor-tropic accumulation exploits differences in blood flow between healthy and tumor vasculature [5]. At the tumor site, the release of the second stage (a polymeric nano-formulation of doxorubicin) is triggered by the acidic tumor environment [4]. To further understand the mechanisms involved in iNPG metastasis accumulation, the aim of this project is to quantitatively analyze the microcirculation in metastatic lungs and characterize their pathophysiology. Microcapillary diameter and blood flow velocity are measured through lung *in vivo* continuous imaging of tumor and healthy vasculature. Paraformaldehyde-fixed fluorescently-labeled red blood cells are used as blood flow trackers. Fluorescent Dextran is used to outline vessel geometry. Home-written MatLab code was developed to systematically measure microcapillary diameters and track velocity from *in vivo* recordings. This code was validated against measurements performed with NikonA1

software. Results from healthy and metastatic lungs were compared to characterize differences in pathophysiology. In the future these results will be used as input for improved iNPG design.

- [1] Nizzero, Sara, et al. "Transport Barriers and Oncophysics in Cancer Treatment." *Trends in Cancer*, vol. 4, no. 4, 2018, pp. 277–280., doi:10.1016/j.trecan.2018.02.008.
- [2] Wilhelm, Stefan, et al. "Analysis of Nanoparticle Delivery to Tumours." *Nature Reviews Materials*, vol. 1, no. 5, 2016, pp. 148–155., doi:10.1038/natrevmats.2016.14.
- [3] Blanco, Elvin, et al. "Principles of Nanoparticle Design for Overcoming Biological Barriers to Drug Delivery." *Nature Biotechnology*, vol. 33, no. 9, 2015, pp. 941–951., doi:10.1038/nbt.3330.
- [4] Xu, Rong, et al. "An Injectable Nanoparticle Generator Enhances Delivery of Cancer Therapeutics." *Nature Biotechnology*, vol. 34, no. 4, 2016, pp. 414–418., doi:10.1038/nbt.3506.
- [5] Van De Ven, Anne L., et al. "Rapid Tumortropic Accumulation of Systemically Injected Plateloid Particles and Their Biodistribution." *Journal of Controlled Release*, vol. 158, no. 1, 2012, pp. 148–155., doi:10.1016/j.jconrel.2011.10.021.

### **O-3.1 - Electrodeposition inhibition of gold nanorods with oxoanions**

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The sensitivity of the localized surface plasmon (LSPR) of gold nanocrystals to changes in the surface chemistry inspires interest in developing applications utilizing the LSPR as a local electrochemical sensor. As the LSPR is directly related to the shape and size of the nanocrystal, changes in these characteristics during electrochemical processes must be understood and controlled. In this study, we demonstrate that the ionic composition of complex electrolyte solutions can significantly influence the morphological stability of gold nanorods (AuNRs) during an electrochemical process. Single particle hyperspectral imaging and correlated scanning electron microscopy show that oxoanions dramatically alter both the dissolution onset potential and the dissolution pathway. Small amounts of bicarbonate and phosphate ions present in predominantly chloride-based electrolyte solutions, for example, inhibit dissolution until increasingly high anodic potentials. Understanding the impact of complex anion solutions on the stability of metal nanocrystal modified electrodes improves capabilities of electrochemical biosensing by increasing the potential window for sensing new species.

### **O-3.2 - STINGel: A Biomaterial-Based Drug Delivery Vehicle for Enhanced Cancer Immunotherapy**

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Modern cancer treatment relies on the discovery and use of potent drug molecules, yet many drugs suffer from inefficient or unoptimized delivery methods. Our work focuses on the development of novel drug delivery vehicles that can be used to enhance the efficacy of existing therapies and treat challenging diseases such as cancer. This is done through the use of Multidomain peptides (MDPs), which can self-assemble into networks of nanofibers that result in injectable hydrogels. Standard MDP hydrogels are biocompatible and can be loaded with various bioactive factors, facilitating cell growth *in vitro* and displaying complete cellular infiltration *in vivo*. This project studies the development of a delivery material to improve the efficacy of STING agonist cyclic dinucleotide (CDN) anti-cancer immunotherapy, taking advantage of the charged domains of a lysine-based MDP hydrogel to achieve extended and localized drug release. The result of this combination of immunotherapy and peptide hydrogel was termed STINGel, and dramatically improves tumor survival over immunotherapy alone in a challenging murine cancer model. Continuing work seeks to develop a second-generation delivery material, by synthesizing and studying new MDPs with different charge chemistries, and by characterizing their effects on drug release kinetics, immune response, and final tumor treatment efficacy. This project's goals are to develop new delivery biomaterials and better drug treatment methods, which will ultimately be translatable to the clinic.

### **O-3.3 - Laser Induced Graphene Multifunctional Composite Surface**

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Fabrication simplification and multi-functionalization are keys for universalization and popularization of current nanomaterials in many fields. Laser Induced Graphene (LIG) is one of the promising candidates in this topic by its one step production with laser ablation of commercial Polyimide (PI) Kapton film under ambient environment and many of its exploding applications. [1] However, LIG potential for realistic applications is limited by the PI substrate it attaches on and its weak robustness. Here, we present a facile infiltration method to fabricate LIG composite surface (LIGCS) compatible with diverse materials that are “Swiss army knife” for multi-purpose applications. We are able to engineer the morphology of several LIGCS to superhydrophobic with contact angle  $> 160^\circ$ . The LIGCS retain the conductivity of the LIG and is suitable for many Joule heating applications, including de-icing and thermal therapy. Stretchable and highly conductive LIGCS is used for resistive memory device substrate and strain sensor. Additionally, LIGCS in constructional materials also show anti-biofouling property.

[1] Lin, Jian, et al. Nature communications 5 (2014): 5714.

### **O-3.4 - Observation of Trochoidal Dichroism**

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Circular dichroism (CD) is the differential extinction of left and right handed circularly polarized light by matter, and CD spectroscopy is ubiquitously utilized for characterization of secondary protein structures and pharmaceutical drugs. While circularly polarized light results when two transverse wave oscillations are out of phase, recent investigations into surface waves, such as those produced by total internal reflection, have revealed wave oscillations in all three dimensions. This includes the surprising property of longitudinal electric field oscillations. When these longitudinal oscillations are out of phase with the in-plane transverse wave oscillations, trochoidal, or cartwheeling, field motion results in the plane. This motion can occur with clockwise or anti-clockwise directionality as a result of the input polarization. In this study, we develop a simple model system whose interaction with light is sensitive to the rotational direction of the electric field in the interface, and we call this polarization sensitivity trochoidal dichroism. We perform single particle spectroscopy of capacitively-coupled orthogonal gold nanorod dimers whose resonance position is sensitive to the rotational motion of the excitation wave. This sensitivity constitutes a geometric basis of polarization sensitivity that fundamentally differs from traditional observations of dichroism that rely only on purely transverse wave oscillations.

### **O-3.5 - Photon Emission by Inelastic Tunneling in Plasmonic Junctions**

Ali Mojibpour,<sup>1</sup> Palash Bharadwaj<sup>1</sup>

Single noble nanoparticle can act as optical antennas, serving as mediating elements between farfield and nearfield optical radiation. While it is most common to generate plasmonic light emission from nanoparticles by optical excitation and scattering, recently there have been reports of electrically excited single nanoparticles. This scheme relies on the principle of inelastic electron tunneling and radiative emission. However, in all previous works the metal nanoparticles were coupled to the metallic electrodes, and light emission resulted from the decay of a strongly excited gap plasmon rather than a true localized surface plasmon resonance (LSPR) of the metal nanoparticle itself. Consequently, the emission wavelength was always redshifted from the LSPR and the quantum yield was affected because of non-radiative coupling to the electrodes.

We present a light emitting tunnel junction where a single noble metal nanoparticle is electrically contacted using graphene electrodes instead of the metallic ones. We choose graphene because it is electrically conducting at low frequencies while presenting a low absorption of only 2.3% per layer at optical frequencies. Indeed, gold nanoparticles in contact with graphene have been shown to experience only a modest increase in their LSPR linewidth due to increase losses to the graphene.

Our scheme allows to achieve electrically driven plasmonic emission from metal nanoparticles made of gold, silver and aluminum, and hence increase the spectral tunability of the plasmonic emission.

### **O-4.1 - Elliptic Path Sampling for Time-of-Flight Rendering**

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During the last decade, we have been witnessing the continued development of new time-of-flight imaging devices, and their increased use in numerous and varied applications. However, physics-based rendering techniques that can accurately simulate these devices are still lacking: existing algorithms exhibit disadvantages such as wasted samples for time-gated cameras and correlational time-of-flight sensors, and non-uniform variance across temporal bins for transient cameras. We take first steps towards addressing these deficiencies, by introducing a procedure for efficiently sampling paths with a predetermined length, and incorporating it within rendering frameworks tailored towards simulating different time-of-flight sensors, such as depth-selective and transient cameras. We use our open-source implementation of the above to empirically demonstrate improved rendering performance in a variety of scenes.

### **O-4.2 - Plasmon-Assisted Ammonia Formation via Chemical Looping**

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The Haber-Bosch process for the industrial manufacture of ammonia (NH<sub>3</sub>) has fundamentally transformed our world by providing fertilizers that allowed the human population to increase from one billion to over seven billion people in the last century. Despite the importance of NH<sub>3</sub>, it remains extremely energy and resource intensive to produce. Annually, the global demand for NH<sub>3</sub> requires 3% of the world's total energy and 5% of the world's natural gas supply, which is compounded by the fact that nearly two tones of CO<sub>2</sub>, a potent anthropogenic greenhouse gas, are produced for every one ton of NH<sub>3</sub>. Here, we describe plasmon-assisted ammonia production via a chemical looping strategy on earth-abundant plasmonic Al-Mg antenna-reactor heterostructures. Chemical looping allows the catalytic formation of ammonia to occur in three distinct steps: (1) nitridation of metallic magnesium (2) hydrolysis of the resulting magnesium nitride to form NH<sub>3</sub> and magnesium oxide and (3) reduction of magnesium oxide back to metallic magnesium to continue the catalytic cycle. Plasmon-assisted chemical looping has several distinct advantages over traditional Haber-Bosch chemistry, such as the ability to use (sun) light as the energy source of the reaction and replacing H<sub>2</sub> traditionally sourced from fossil fuels with H<sub>2</sub>O for the formation of NH<sub>3</sub>. This plasmon-assisted process also greatly lowers the operating temperatures and pressures, suggesting that plasmon-assisted ammonia formation via chemical looping could become a sustainable alternative to the standard model for NH<sub>3</sub> production.

### **O-4.3 - Washable ECG Electrodes from Sewn High Performance Carbon Nanotube Fibers**

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Commercially available electrocardiogram (ECG) electrodes are rigid and require a gel electrolyte to obtain a proper signal. This electrolyte can dry over time leading to a degradation in signal to noise ratio. Furthermore, the lack of airflow to the skin and adhesive can be irritating to the user. This can pose issues for individuals that require continuous monitoring. Here, we present ECG electrodes made with high performance carbon nanotube (CNT) fiber that are suitable for long-term use. The high conductivity of the fiber and low contact impedance between the fiber and skin allow for good transmission of the ECG signal without the use of a gel. Additionally, the CNT fiber has excellent tensile strength and flexibility so it can be sewn into fabric with a standard sewing machine. The woven structure and softness minimizes the irritation caused by recording ECGs. Finally, the CNT fiber is robust and chemically inert so that it can be machine washed without losing performance.

#### **O-4.4 - Probing interfacial bovine serum albumin unfolding with single molecule high resolution imaging with photobleaching**

Lauren Warning,<sup>1</sup> Rashad Baiyasi,<sup>2</sup> Qingfeng Zhang,<sup>1</sup> Sudeshna Chatterjee,<sup>1</sup> Nicholas Moringo,<sup>1</sup> Joey Tauzin,<sup>1</sup> Christy Landes,<sup>1,2</sup> and Stephan Link<sup>1,2</sup>

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Understanding the protein conformational changes at solid-liquid interfaces is critical for predicting how proteins will impact the performance of *in vivo* biomaterials. Single molecule fluorescence microscopy strategies are advantageous for directly probing protein unfolding, in which the intra-dye distance between two emitters attached to the same protein is measured; greater intra-dye distances indicate a greater degree of unfolding. While single molecule Förster Resonance Energy Transfer is most commonly used to characterize protein unfolding, it is limited to inter-dye distances up to about 10 nm, and it requires dye labeling specificity that is complicated for many biologically relevant proteins. In the current work, we develop the use of single molecule high resolution imaging with photobleaching, a localization-based analysis strategy, to quantify the intra-dye distances of single multi-dye-labeled bovine serum albumin (BSA) proteins adsorbed to glass. With this technique, we can measure distances 5 nm and beyond using commercially available dye-conjugated proteins. Preliminary results indicate that BSA does unfold at the solid interface, and ongoing work, such as exploring how conditions such as protein crowding, surface chemistry, and charge shielding affect BSA's conformation on surfaces, will be discussed.

#### **O-4.5 - Compressive Hyperspectral Microscopy of Nanomaterials**

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Imaging with hyperspectral microscopy using conventional techniques typically involves a trade-off between resolution, acquisition time, and expense due to a combination of low pixel-by-pixel signal intensity and detector sensitivity. In this work, we applied compressive sensing theory to hyperspectral microscopy. The combination of compressive light modulation with sparsity-based reconstruction algorithms enhances the measurement signal-to-noise ratio and allows for rapid acquisition of the full spectrum at every pixel in the image, even though the total hypercube is sub-sampled. We present the successful demonstration in dark field and bright field

transmission imaging modality. The utility of this approach is demonstrated by measuring the plasmon resonance spectra of single gold nanoparticles and comparing the spectra with those measured by an expensive commercialized push-broom spectrometer. The result verifies that the proposed technique produces the same spectra of nanoparticles as the push-broom spectrometer, with added advantages of a lower cost and shorter measurement time. We also demonstrate the application of this technique to characterizing the optoelectronic properties of two-dimensional transition metal dichalcogenide thin films and nanoflakes.



**GP-A Poster Session**

**GP-A-01 Transition of Surfactant Structure Surrounding Gold Nanorods by Analytic Surface-Enhanced Raman Scattering**

Aobo Zhang,<sup>1</sup> Steven M. E. Demers,<sup>1</sup> Jason H. Hafner,<sup>1,2</sup> Louis E. Cole<sup>1</sup>

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The surfactant cetyltrimethylammonium bromide (CTAB) plays an important role in the synthesis of gold nanoparticles from gold chloride solutions. The CTAB layer surrounding gold nanoparticles prevents them from aggregating so it can direct the synthesis to form specific nanoparticle shapes. The structure of CTAB layer is of great interest to understand the synthesis processes and improve gold nanoparticle production and modification techniques.

A structural transition of the CTAB layer is observed by a new structure analysis method based on surface-enhanced Raman (SERS) and unenhanced Raman spectroscopy. The new method analytically takes ratios of SERS and Raman peaks of CTAB vibration modes. The tilted angle of alkane chains can be calculated with the help of Raman tensors from time-dependent density functional theory (TDDFT) and enhanced electric field by COMSOL simulation. The tilted angle is found to be 27° when there are sufficient CTAB molecules to form a stable layer. After the CTAB concentration is lowered to 3-4mM, the analysis indicates an increased angle. The changing of tilted angle indicates the collapse of CTAB layer and the formation of new CTAB structure.

**GP-A-02 Protein Folding, Binding and Aggregation in the Cell: Role of Stochastic Resonance**

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Understanding how proteins fold and form multi-protein assemblies inside the cell is an important fundamental problem that has vital implications for development of therapeutic methods. The cellular environment is critically different from the dilute and static conditions under which proteins are usually studied in vitro or using computational approaches. Protein folding and protein-protein binding inside the cell occur in highly crowded and fluctuating environment, which is critical for stability of larger proteins and assemblies. While, the role of crowding has been extensively investigated previously, the role of fluctuations has been largely neglected. Here, we report on our investigation into the role of local fluctuations that can be attributed to fluctuations of the chemical environment around the protein inside the cell. Using coarse-grained molecular simulations we establish that such fluctuations can have a substantial effect when the characteristic frequency of the applied fluctuations coincides with the “native” rates of the reaction, consistent with the phenomenon of stochastic resonance observed in many other condensed-matter processes. Our computational and theoretical findings as well as the recent experimental conformation of our results will be presented.

**GP-A-03 Microfluidic actuation of flexible microelectrodes for neural recording**

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Electrical neural recording could help reveal how information transfer between neurons contributes to underlying brain functions and behaviors. Flexible polymer-based microelectrodes cause less tissue damage and show better reliability and longevity compared to conventional Si-based microelectrodes and metallic microwires. However, this flexible nature necessitates stiffeners or shuttle devices to assist insertion into the brain, which increases the implant footprint and causes more acute damage to the tissue no matter how small the shuttle device is. Recently, we developed a method of microfluidics-assisted insertion of flexible microelectrodes for neural recording. A drive channel in the fluidic microdrive provides mechanical support, then a bio-compatible viscous liquid is flowed to push the flexible microelectrode into the brain, with no increase in the footprint of the microelectrode itself. Two vent ports allow the flexible microelectrodes to move forward with minimal liquid following to the brain. Our current efforts focus on comparing the tissue damage in *in vivo* implantation between microfluidics-assisted and stiffener-assisted flexible microelectrodes insertion.

### **GP-A-04 Improved structural prediction of peptide-HLA complexes using DINC-Vina**

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Immunotherapy makes use of the patient's own immune system to identify and eliminate cancer cells, representing a promising new avenue for cancer treatment. The class I human leukocyte antigen (HLA) receptors play a key role in this context, binding and displaying at the cell surface peptides derived from intracellular proteins. These peptide-HLA complexes can be recognized by circulating T-cell lymphocytes, triggering T-cell activation and tumor elimination. T-cell activation is driven by intramolecular interactions, and structural analyses of peptide-HLA complexes are becoming essential for the development of new T-cell-based immunotherapies. In this context, we previously proposed an incremental meta-docking approach called DINC, and provided preliminary data supporting its use for general prediction of binding modes of peptide-HLA complexes. Here we describe improved prediction of peptide-HLA complexes using DINC-Vina (using AutoDock Vina). For that, we report a re-docking experiment aiming to reproduce a diverse dataset of peptide-HLA complexes available in the Protein Data Bank. Our method is able to reproduce all complexes with less than 2 Å all-atom RMSD (with an average of  $1.33 \pm 0.3$  Å across the whole dataset). Our new method also shows improved reproducibility, with high consistency of low RMSD conformations across 20 replicates of the same experiment. On the other hand, consistency in terms of the top scoring conformation has proven to be a much bigger challenge. Future development of DINC-Vina will allow fast and accurate geometry prediction of patient-specific peptide-HLA complexes. In turn, these predictions will have a positive impact on personalized T-cell-based immunotherapies against cancer.

### **GP-A-05 Aluminum nanocrystals @ metal-organic frameworks: a new addition for sustainable plasmonics**

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Metal organic frameworks (MOFs) and metal nanoparticles are two classes of materials that have received considerable recent attention, each for controlling chemical reactivities, but in very different ways. Here, we report the

growth of MOF shell layers surrounding Al nanocrystals, an earth-abundant metal with energetic, plasmonic and photocatalytic properties. The MOF shell growth proceeds by means of a unique dissolution-and-growth chemistry that utilizes the intrinsic surface oxide of the nanocrystal to obtain the Al<sup>3+</sup> ions accommodated into the MOF nodes. Changes in the Al nanocrystal plasmon resonance provide an intrinsic optical probe of its dissolution and growth kinetics. This same chemistry enables a highly controlled oxidation of the Al nanocrystal, providing a precise method for reducing nanocrystal size in a shape-preserving manner. MOF shell encapsulation of the Al nanocrystal results in increased efficiencies for plasmon-enhanced photocatalysis, observed for the hydrogen-deuterium exchange and reverse water-gas shift reactions. MOF growth around Al nanocrystals provides a new level of control over both Al nanocrystal growth chemistry and its photocatalytic reactivity.

## **GP-A-06 Optical Force Reshaping of Au Nanodisks in Al-Au Heterodimers**

Jian Yang,<sup>1,2</sup> Chao Zhang,<sup>2,3</sup> Thejaswi Tumkur,<sup>2,3</sup> Minhan Lou<sup>2,3</sup>, Liangliang Dong<sup>3,4</sup>, Linan Zhou<sup>3,4</sup>, Peter Nordlander<sup>1,2,3,5</sup>, and Naomi J. Halas<sup>1,2,3,4,5</sup> \*

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The optical reshaping of metallic nanostructures typically requires intense laser pulses to first approach or achieve melting, followed by surface-tension-dominated reshaping, transforming the original nanostructures into more spherical morphologies. Here we report the observation of optical reshaping of Au nanodisks in Al-Au heterodimers under direct illumination, in the junction of a photo-induced optical force microscope, where a reshaping of only the Au nanodisk component of the heterodimer occurs. There are three contributors to this process: a photothermal softening of the Au lattice, the optical forces applied to the Au nanodisk by the Al nanodisk, and also by the nearby AFM tip. The asymmetric reshaping of the heterodimer is observable structurally, through electron microscopic imaging, and through changes in the heterodimer optical response. This optical force-directed shape manipulation may have potential applications in nanofabrication, optically-induced nanomanufacturing, sensing, and quality control.

## **GP-A-07 Magnetolectric materials for miniature, wireless neural stimulation in freely behaving animals**

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Miniature, wireless neural stimulators would improve our ability to treat disease and allow for easier access to brain regions and peripheral nerves that are difficult to address using wired devices. In particular, miniaturization is critical to reduce the invasiveness of bioelectronic implants; however, efficient wireless power transfer through bone and tissue to enable neurostimulation in deeply implanted millimeter sized devices remains a major challenge. Furthermore, the capability to produce charge-balanced, biphasic stimulation is particularly difficult in miniaturized designs and has not yet been demonstrated in freely moving animals without the use of batteries or inductive coils that significantly increase the device footprint. Here we show that millimeter sized magnetolectric (ME) materials can be wirelessly powered using alternating magnetic fields that match acoustic resonant modes of the material. When driven at resonance, these materials generate sufficient voltage to stimulate neurons both *in vitro* and *in vivo*. The major advantage of this approach is the fact that the magnetic fields in this frequency range (10-500 kHz) are nearly unattenuated by bone and tissue. Based on this principle, we demonstrate the smallest and lightest biphasic wireless stimulator in a freely moving animal by selectively activating two different ME films on the same device. Furthermore, we find that the voltages generated by these films

remain sufficiently large as the films are made smaller, suggesting that ME materials are an excellent candidate for wirelessly powering miniature charge-balanced neural stimulators.

## **GP-A-08 The Effects of Charge State on the Lifetime Dynamics of Plasmons in the Few-Atom Limit**

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Graphene has been shown to be an exceptional material for supporting plasmons, with a tunability ranging from the mid-infrared to terahertz frequencies. Here we consider polycyclic aromatic hydrocarbon (PAH) molecules as essentially graphene nanoislands in the quantum limit, typically consisting of 50 or fewer atoms. With the addition or removal of even a single electron, it has been shown these molecules can still support molecular plasmon (collective) resonances pushed into the visible region of the spectrum. We have thus probed the plasmon dynamics in these quantum systems by measuring the excited state lifetime of several PAH molecules in four different charge states: the cation, neutral, anion, and dianion states. Molecules in their neutral or dianion states (closed-shell) were found to exhibit long-lived mono-exponential decays typical of molecular radiative relaxation and indicative of single-electron excitation dynamics. In contrast, molecules in their cation and anion states (open-shell) exhibit far more rapid multi-exponential decay dynamics attributed to the de-excitation of multiple electron-hole pairs through molecular plasmon “dephasing” and vibrational relaxation of the molecule. This study provides a look into the distinction between collective and single-electron excitation dynamics in the purely quantum limit and helps illuminate what electronic structure in a molecule can support such dynamics.

## **GP-A-09 Structural Analysis of Ibuprofen and Ovispirin-1 in Lipid Bilayer**

Mathieu Simeral, Lee Hsieh

Abstract

In this research, we use surface enhanced Raman scattering (SERS) to determine the orientation of a nonsteroidal inflammatory drug (NSAID), ibuprofen molecule, and ovispirin-1 within a lipid bilayer. Gold rods under proper illumination create intense electric fields at their ends. This leads to SERS from molecules located at the ends of the rods that carries information about their location and orientation with respect to the rods. A method previously described by our group<sup>1</sup> uses SERS spectra as well as computational results for the polarizability of the molecule of interest, and electromagnetic near fields to extract information about its orientation. We apply this structural analysis by enhanced Raman scattering (SABERS) method to ibuprofen within a phospholipid bilayer on a gold nanorod, as well as ovispirin-1 within a phospholipid bilayer.

<sup>1</sup> **Structural Analysis by Enhanced Raman Scattering**  
James R. Matthews, Cyna R. Shirazinejad, Grace A. Isakson, Steven M. E. Demers, and Jason H. Hafner  
*Nano Letters* **2017** 17 (4), 2172-2177  
DOI: 10.1021/acs.nanolett.6b04509

## **GP-A-10 The three-dimensional architecture of the human genome: it's nuclear physics!**

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The human genome is composed of 46 DNA molecules — the chromosomes — with a combined length of about 2 meters. Chromosomes are stored in the cell nucleus in a very organized fashion that is specific to the cell type; this three-dimensional architecture is a key element of transcriptional regulation and its disruption often leads to disease. What is the physical mechanism leading to genome architecture? If the DNA contained in every human cell is identical, where is the information — the blueprint — of such architecture stored?

In a series of works, we were able to demonstrate that the architecture of interphase chromosomes is encoded in the one-dimensional sequence of epigenetic markings much as three-dimensional protein structures are determined by their one-dimensional sequence of amino acids. In contrast to the situation for proteins, however, the sequence code provided by the epigenetic marks decorating the chromatin fiber is not fixed but is dynamically rewritten during cell differentiation, modulating both the three-dimensional structure and gene expression in different cell types.

*In vivo*, segments of chromatin characterized by homogeneous epigenetic markings undergo a process similar to phase separation under the action of the proteome present in the nucleus. This process forms liquid droplets, which rearrange dynamically by splitting and fusing, thereby modulating DNA distal interactions and generating the genomic compartments characteristic of chromosomal architecture.

Our theory — together with our computational tools — allows predicting and studying the spatial conformation of genomes with unprecedented accuracy and specificity, thus opening the way to the study of the functional aspects of genome architecture.

## ***GP-A-11* Investigating the Effect of Anti-cancer Compound (Piperlongumine) on the Physical Properties of Cancer Cells Using Atomic Force Microscopy**

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Natural compounds have shown a great potential for cancer treatment. Piperlongumine (PL), a natural anti-tumor compound derived from pepper species, has been demonstrated anti-cancer effect on HeLa cells, and toxicity of PL against HeLa cells has been investigated. Here we focus on understanding the mechanical properties of HeLa cells under PL treatment, using Atomic Force Microscopy (AFM) based single-cell manipulation technique. We used AFM to pull single HeLa cells and acquired the force-distance curve. The characteristic force curves showed stepwise patterns, and we analyzed the step force and found that, that under treatment of PL, the most probable step force shifted to higher values compared to the non-treated cells. This change was observed in cells on substrates of different stiffness. These effects may be due to the change in cytoskeleton structure of HeLa cells after PL treatment, possibly due to microtubule destabilization by PL. Therefore, understanding the PL effects on the cellular physical properties beyond the biochemical mechanisms of PL's anti-cancer effects, may help in the development of effective therapeutic drugs against cancers.

This work was supported by Conselho Nac. Des. Cient. Tecnológico (CNPq # 141714/2017-4), Prog. Pós-Graduação Unesp (PROPG-Unesp), and the Welch Foundation (C-1632).

## ***GP-A-12* Structure-Dependent Multimodal Transport of Transferrin on Nylon Supports**

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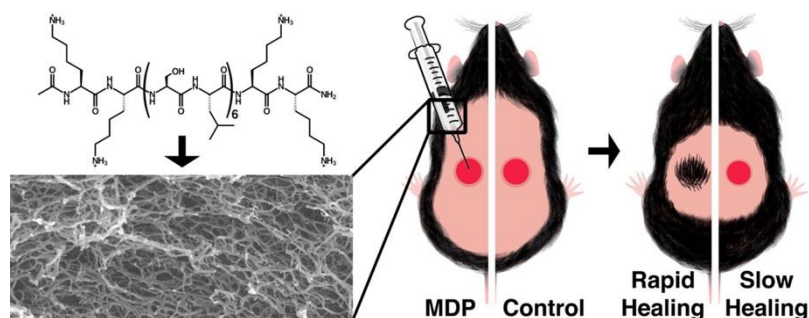
Current downstream costs of pharmaceutical drug separations consume 50% of the \$2.6 billion to bring a promising therapeutic drug to market. Industrial separations heavily rely on empirically driven chromatographic separations. This large financial burden on drug development originates from a knowledge gap in protein mass transport in chromatographic columns. In particular, the highly dynamic and multiplexed interfacial interactions of target protein and supporting stationary phase materials is experimentally challenging to monitor *in situ*. Here single molecule tracking is utilized to track single protein molecules below the diffraction limit of light in real time to provide a mechanistic understanding of surface transport and the relation to ensemble separations. Results indicate the protein separation of a model protein transferrin was dependent on the structural confirmation of our model protein including the surface transport dynamics varied at different ionic concentrations.

### **GP-A-13    Multidomain Peptide Hydrogel Accelerates Healing of Full-Thickness Wounds in Diabetic Mice**

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Multidomain peptide (MDP) hydrogels are a class of self-assembling peptides. The peptide sequence contains a core of alternating hydrophilic and hydrophobic amino acids flanked by charged amino acids. This design triggers formation of a beta-sheet secondary structure, resulting in a facial amphiphile. In aqueous solutions, the hydrophobic effect leads to self-assembly of the peptides into nanofibers stabilized by hydrogen bonding between adjacent peptide backbones. The addition of multivalent salts, such as those found in common buffers, allows nanofiber elongation and cross-linking to form a viscoelastic hydrogel. MDPs are cytocompatible and support cell growth and proliferation *in vitro*. *In vivo*, MDP hydrogels are capable of rapid cellular infiltration and produce a mild inflammatory response leading to the formation of blood vessels. Over time, the nanofibers of the MDP hydrogel are degraded and replaced by a natural collagen-based extracellular matrix effectively remodeling the artificial material into native tissue. These properties make MDPs particularly well suited for applications in tissue regeneration. In this work, the regenerative potential of MDP hydrogels in a diabetic wound healing model was explored. When applied to full-thickness dermal wounds in genetically diabetic mice, the MDP hydrogel results in significantly accelerated wound healing compared to a clinically used hydrogel, as well as a control buffer. Treatment with the MDP hydrogel resulted in wound closure in 14 days, formation of thick granulation tissue within the wound space with the presence of dense vascularization, innervation by the peripheral nervous system, and hair follicle regeneration.



## **GP-A-14 Designing Nonspecific Sensors for the Scalable Identification of Microbes**

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The rapid identification of microbes has broad applications in clinical diagnostics. The majority of current molecular diagnostics are target-specific, necessitating a unique sensor for every possible microbial species in the sample. Our previous research demonstrated that a relatively small set of random DNA probes that bind nonspecifically at several locations on the genomes of target species could distinguish the microbes by giving each its own signature binding profile to the probes. Here, we present a genetic algorithm that deterministically designs locally optimal DNA probes for a given list of targets by iteratively mutating the probes towards those that maximize the difference in their binding profiles. This algorithm is enabled by a rapid heuristic that we developed for the overall binding strength between an arbitrary probe and target genome. We represented sequences as “bags-of-words,” where the words are short subsequences of DNA, allowing arbitrarily long sequences to be condensed into equal length vectors. The inner product between the bag-of-words representations of a probe and genome correlates with the results of advanced thermodynamic simulations (generally  $R^2 > 0.8$ ) and is computed in milliseconds. With the wealth of publicly available microbial sequence data, the scope of possible applications for our system is enormous, and our flexible algorithm will enable the judicious selection of the most promising avenues to pursue. We present two preliminary sets of designed probes for applications in the diagnosis of bacterial infections and the assessment of gut microbiome composition.

## **GP-A-15 PSF Distortion in Dye – Plasmonic Nanomaterial Systems: Friend or Foe?**

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Plasmonic nanostructures offer promising applications as nanocatalysts, but optimizing their structure-function relationship using optical superlocalization techniques is hindered by the formation of distorted point spread functions. Previously reported localization bias for remotely excited Alexa-647 adsorbed to Ag nanowires is investigated here for its potential to provide useful information about surface interactions. Two main classes of abnormal PSFs are examined: single-lobed PSFs in which the localization bias arises from various emitter positions around the nanowire, and bi-lobed PSFs arising from emitters near the top edge of the nanowire. The amount of localization bias for these two populations diverges for ground truth widths less than 300 nm, and suggests the corresponding adsorption and resulting orientation arise more frequently under experimental conditions than is predicted by simulation. Nanowires with widths in the range of 200 to 300 nm are found to have the greatest potential for distinguishing between single-lobed and bi-lobed PSFs in experiment. Finally, we present a fitting method for abnormal PSFs using a basis of Hermite-Gaussian functions and show that orientation information is encoded in bi-lobed PSFs. Future work focusing on detecting and localizing abnormal PSFs will enable the use of superlocalization techniques to identify and track fluorescent dyes and other quantum emitters on plasmonic nanowires.

## **GP-A-16 The Effect of Charged-Pair Interactions on the Stability of the Collagen Triple Helix**

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Collagen is one of the most prevalent molecules in the human body; thus, it is important to understand the stability and structure of this important protein. Due to the heterogeneity and poor solubility of natural collagen, collagen mimetic peptides (CMPs) are frequently used to study structural characteristics of the protein in a controlled environment. CMPs are made up of three strands forming a triple helix, each strand contains the triplet motif (Xaa-Yaa-Gly)<sub>n</sub> with Xaa frequently being proline and Yaa being hydroxyproline. The triple helix is stabilized by hydrogen bonds on the inside between the peptide backbones and by charged-pair interactions on the outside between amino acid side chains. In order for a charged-pair interaction to occur along the CMP, the amino acid side chains must obtain specific geometries. Two known geometries are termed “axial interactions” and “lateral interactions.” In this study, the axial and lateral interaction geometries are compared to determine the difference in contributions to the collagen triple helix stability using Circular Dichroism Spectroscopy and NMR. The comparison of conformations shows axial interactions confer greater stability to the collagen triple helix, while lateral interactions contribute little stability, and single substitutions are considered destabilizing.

### **GP-A-17 Charge transfer between gold nanorods and electropolymerized metal complex nano-coatings**

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Optically and electronically coupling coordination complex catalysts to plasmonic nanoantennas can achieve higher selectivities and efficiencies for photocatalytic chemical transformations than each component can yield individually. Here we show that a conductive coating of poly-nickel(II) tetra(amino)phthalocyanine can be electropolymerized selectively from individual gold nanorod electrodes on supporting indium tin oxide films, producing optically and electronically coupled antenna-polymeric hybrid nanostructures. We demonstrate with in situ spectroelectrochemical dark-field microscopy that the sequential growth of the organometallic polymer can be tracked on multiple individual gold nanorods by recording hyperspectral scattering images. Selective growth of the polymer was achieved by using a low monomer concentration of 10 μM and a low cyclic voltammetry anodic limit of 400 mV. The polymer coating thickness and heterogeneity was characterized using scanning electron microscopy analysis. Our optical spectroscopy results show that for gold nanorods with average dimensions of 40 nm × 70 nm the average localized surface plasmon resonance energy and intensity decreased by 50 meV and 50%, respectively, and the resonance linewidth increased by 150 meV, with the growth of a 20 nm polymer coating. The observed linewidth increase with the addition of the polymer coating is the effect of a greatly decreased dephasing time of the plasmon. We propose the decrease in plasmon dephasing time is because the phthalocyanine ligands have a high density of unoccupied molecular orbitals close to the resonance energy that can readily accept hot electrons across the antenna-polymer interface.

### **GP-A-18 Al@TiO<sub>2</sub> Nanoshell: Synthesis, Water Tolerance and Photocatalysis**

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Al nanocrystals (Al NCs) have shown excellent plasmonic properties from UV to visible region. However, its application in aqueous environment is limited by the poor water stability. TiO<sub>2</sub>, as a commonly used photocatalyst, shows extraordinary performance under UV light. To improve the water stability of Al NCs in aqueous environment and to



enhance the performance of TiO<sub>2</sub> under UV light, core-shell Al@TiO<sub>2</sub> nanoparticles were successfully synthesized. Using TiOSO<sub>4</sub> in H<sub>2</sub>SO<sub>4</sub> solution as precursor, the native oxide layer on Al NCs were etched off while the coating of TiO(OH)<sub>2</sub> occurred. Anatase TiO<sub>2</sub> shell is formed after annealing. There is an interlayer at Al/TiO<sub>2</sub> interface, confirmed by The Al@TiO<sub>2</sub> core-shell structure showed excellent water stability under 30 days. The degradation of methylene blue (MB) confirmed that Al@TiO<sub>2</sub> is a promising photocatalyst.

## **GP-A-19 Phosphorylation induces conformational rigidity at the C-terminal domain of AMPA receptors**

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Ionotropic glutamate receptors serve as ion channels in the neuronal membrane and are responsible for fast excitatory neurotransmission across synapses in our central nervous system. Among the four different domains of glutamate receptors, the intracellular C-terminal domain (CTD) is the most difficult to crystallize. Thus, structural and dynamic properties of the CTD are less investigated. CTD of AMPA receptor undergoes phosphorylation at specific locations during long-term potentiation (LTP) and results in enhancement of channel conductance. However, conformational changes caused by phosphorylation has not been studied well, leaving a gap in elucidating the mechanism associated with it. Herein, single molecule Förster resonance energy transfer (smFRET) has been used as a spectroscopic probe of conformational changes of a section of CTD under the conditions of phosphomimicry. The results from this study show that phosphomimicry induces conformational rigidity to the CTD and such conformational changes are essentially an electrostatic effect.

## **GP-A-20 Database of Transmission (T), Absorbance (A), and Reflectance (R) for 2-Dimensional Materials**

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Despite being only a few atoms thick, single-layer two-dimensional (2D) materials display strong electron-photon interactions that could be utilized in efficient light modulators on extreme subwavelength scales. In various applications involving light modulation and manipulation, materials with strong optical response at different wavelengths are required. We using first-principles calculations create a database of 2D materials to seek out candidates with strongest optical response in various frequency ranges, from mid-infrared (IR) to deep ultraviolet (UV). We find that 2D boron has broadband reflectance  $R > 99\%$  for  $>100$  layers, surpassing conventional thin films of bulk metals such as silver. Moreover, 2D semiconductors are found to show intriguing absorbance for which, we obtain quantitative estimates by calculating quasiparticle energies and accounting for excitonic effects by solving the Bethe-Salpeter equation (BSE). We identify several monolayer semiconductors with absorbances  $\geq 30\%$  in different optical ranges which are more than half of the maximum possible value for a 2D material. Our study predicts 2D materials which can potentially be used in ultra-thin reflectors and absorbers for optoelectronic application in various frequency ranges.

## **GP-A-21 Investigating Gold Nanoparticle Shape and Size Dependence for Electrogenerated Chemiluminescence**

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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)<sub>3</sub><sup>2+</sup> with coreactant tripropylamine. Depending on the spectral overlap of the ECL emission and the adsorption of the nanoparticle, some enhancement in ECL intensity may be observable due to a decreased emission lifetime. The work presented shows initial studies into the effect of nanoparticle shape and size on surface area normalized ECL intensity.

## **GP-A-22 Ultrastiff Graphene Foams as Three-Dimensional Conductive Fillers for Epoxy Resin**

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Conductive epoxy composites are of great interest due to their applications in electronics. They are usually made by mixing powdered conductive fillers with epoxy. But the conductivity of the composite is limited by the low filler content because increasing filler content causes processing difficulties and reduces the mechanical properties of the epoxy host. We present here a dense enough 3D filler material – ultrastiff graphene foams synthesized from polyacrylonitrile by the power metallurgy method – for epoxy resin. The foams have a density of 0.3-0.4 g/cm<sup>3</sup>, which is at least 4 times higher than most of the conventional graphene foams prepared by CVD, hydrothermal reaction, or freeze-drying. The high density renders the foams with remarkable mechanical strength and electrical conductivity. Use of these foams not only improve the electrical conductivity of epoxy to an unprecedented level (41.0 ± 6.3 S/cm) that is even comparable to the conductive polymer matrices reported to date, but increase the compressive modulus of epoxy by ~1732%! Additionally, the density of the composite only goes up by 8%. We have demonstrated the distinct advantages of this ultrastiff 3D graphene foams over all powdered fillers and conventional 3D fillers.

## **GP-A-23 Vacuum Bloch-Siegert Shift in Landau Polaritons with Ultrahigh Cooperativity**

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Geoff Gardner,<sup>4</sup> Weilu Gao,<sup>1</sup> Minhan Lou,<sup>1</sup> Katsumasa Yoshioka,<sup>5</sup>  
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A two-level system resonantly interacting with an ac magnetic or electric field constitutes the physical basis of diverse phenomena and technologies, including nuclear magnetic resonance, stimulated emission, amplification, Rabi oscillations, laser cooling, and quantum information processing. However, despite the seeming simplicity of the problem, Schrödinger's equation for this system can be solved exactly only under the rotating wave approximation, which neglects the counter-rotating field component. When the ac field is sufficiently strong, this approximation fails, leading to a resonance-frequency shift known as the Bloch-Siegert (BS) shift, which is typically minuscule and difficult to analyze. Here, we report the vacuum BS shift, which is induced by the ultrastrong coupling of matter with the counter-rotating component of the vacuum fluctuation field in a cavity. Specifically, an ultrahigh-mobility 2D electron gas inside a high-Q terahertz cavity in a quantizing magnetic field revealed Landau polaritons with a record high value (3513) of the ratio of the vacuum Rabi splitting to the polariton linewidth. Unlike the usual BS shift, we observed an unambiguously large vacuum BS shift up to 40 GHz, which can be exactly analyzed as a consequence of the ultrastrong coupling of counter-rotating circularly polarized radiation and Landau-quantized electrons. This shift, clearly distinguishable from the photon-field self-interaction effect, represents a unique manifestation of a strong-field phenomenon without a strong field.

### **GP-A-24 Hydrogen peroxide production from hydroxylamine using palladium-decorated gold nanoparticle**

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Hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) is widely used in daily life and industry. It is produced in large scale by the anthraquinone oxidation (AO) process. However, this process involves the use of organic solvent and energy-intensive liquid-liquid extraction to recover H<sub>2</sub>O<sub>2</sub>, which is not a green process and cost-effective. Thus, novel and greener methods for the production of H<sub>2</sub>O<sub>2</sub> were explored. The direct synthesis of H<sub>2</sub>O<sub>2</sub> from O<sub>2</sub> and H<sub>2</sub> gas using a variety of catalysts were reported, but these processes were possibly explosive and not safe for industrial operation. In this study, instead of using H<sub>2</sub> gas, we used a relatively safe liquid-phase hydrogen donor chemical - hydroxylamine to produce H<sub>2</sub>O<sub>2</sub>. In our process, the rapid and selective production of H<sub>2</sub>O<sub>2</sub> can be achieved by the use of unique designed Pd-decorated Au catalysts.

### **GP-A-25 Tailoring the Properties of Single-Wall Carbon Nanotube Samples through Structure-Selective Photochemistry**

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As-produced samples of single-wall carbon nanotubes (SWCNTs) contain many structural forms with different optical, electronic, and physical properties. A major and challenging goal in this field is sorting or

tailoring the properties of these mixtures for basic research studies and applications. We will present promising early results from a new approach that uses monochromatic near-infrared light to induce structure-selective photochemistry in mixed samples.

We have discovered that dissolved molecular oxygen reacts with semiconducting SWCNTs that have been irradiated at their lowest energy electronic absorption ( $E_{11}$ ). The reacted SWCNTs show strong permanent quenching of their fluorescence emission while other nanotubes in the sample remain largely unaffected. Laser irradiation at 955, 985, and 1130 nm selectively quenches emission from (8,3), (6,5) and (7,6) nanotubes, respectively. The photoreaction depends monotonically on the concentration of dissolved  $O_2$ . We have characterized the reacting samples using fluorescence, absorption, and Raman spectroscopies. The role of surfactant coating has also been studied for SWCNTs dispersed in aqueous pluronic-F127, sodium dodecyl sulfate, sodium dodecylbenzenesulfonate and single-stranded DNA. Ongoing studies are investigating selective photochemistry with other reactants. We believe that this work opens an important new route for controlling the properties and compositions of SWCNT samples.

## **GP-B Poster Session**

### ***GP-B-01* Active Control of Protein Dynamics on Interfaces**

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**Abstract:** Active control of protein or biomolecule interactions on surfaces is desired for various real-life applications in a diverse field of interests, ranging from drug delivery, biosensors, protein and biomolecule separation and purification. Physio-chemically cross-linked hydrogel particles made of stimuli-responsive smart polymers have attracted considerable attention in recent years. Nanoscale hydrogel particles dispersed in aqueous medium or ‘nanogels’ are soft nanomaterials that display variable physio-chemical character at various environments. Nanogels of poly(N-isopropylacrylamide) (PNIPAM) functionalized with allyl amine (AA) groups respond to external pH change by changing their size and electrostatic nature of the surface.

Fluorescence based single molecule microscopy and single particle tracking methods are ideal to understand the complex dynamic behavior of proteins at the polymer surface. In this study, the dynamics of a model protein lysozyme on the pH- responsive PNIPAM-co-AA nanogel surface and inside the nanogel cavity were investigated at various environmental conditions using single molecule methods. We present a molecular level understanding of the specific interactions between nanogel particles and proteins. Understanding these complex surface and intra-cavity dynamics of biomolecules will instigate further theoretical and experimental studies of these systems. This will inspire better bottom-up design strategies with other stimuli-responsive polymers for various applications including, but not limited to, separation science and biomedical sciences.

### ***GP-B-02* Controlling Chemistry with Light**

Linan Zhou,<sup>1</sup> Dayne F. Swearer,<sup>1</sup> Chao Zhang,<sup>2</sup> Hossein Robotjazi,<sup>2</sup> Hangqi Zhao,<sup>2</sup> Luke Henderson,<sup>1</sup> Liangliang Dong,<sup>1</sup> Phillip Christopher,<sup>3</sup> Emily A. Carter,<sup>4</sup> Peter Nordlander,<sup>2,5\*</sup> and Naomi J. Halas<sup>1,2,5\*</sup>

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Photocatalysis based on optically active, “plasmonic” metal nanoparticles has emerged as a promising approach to facilitate light-driven chemical conversions under far milder conditions than thermal catalysis. In plasmonic photocatalysis, both hot-carrier-driven process and photothermal heating effect contribute to enhance chemical reactions. But an understanding of the relation between thermal and electronic excitations has been lacking.

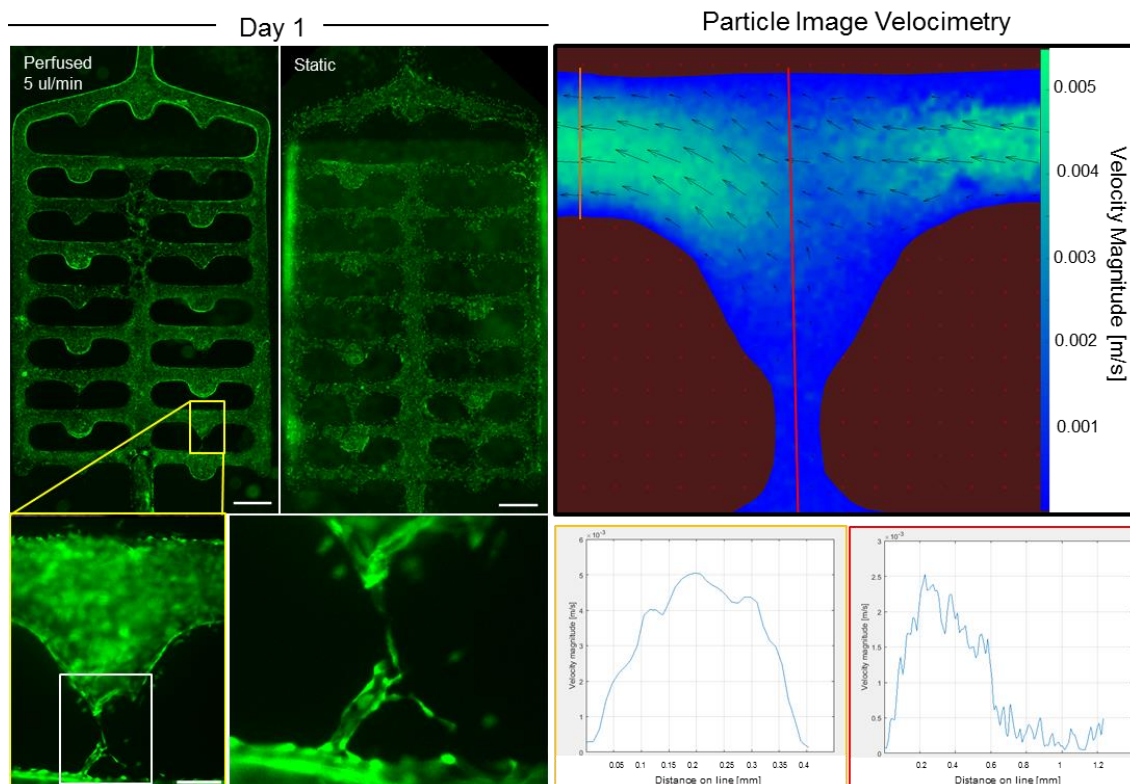
We reported the substantial light-induced reduction, as much as 1 eV, of the thermal activation barrier of ammonia decomposition on a plasmonic photocatalyst by light excitation and the concomitant high energy efficiency of 18% in photocatalysis. We systematically studied the effects of optical illumination on the apparent activation barrier  $E_a$  for  $\text{NH}_3$  decomposition ( $2\text{NH}_3 \rightarrow \text{N}_2 + 3\text{H}_2$ ) using a plasmonic antenna-reactor photocatalyst. Our analysis showed that photoinduced reductions of the reaction barrier have an electronic origin. Further study on reaction kinetics revealed that hot-carrier excitation lowered the  $E_a$  by preferably activating the rate-limiting step, namely combinative desorption of  $\text{N}_2$ , probably through the Desorption Induced by Electronic Transitions (DIET) mechanism, and changed the reaction energetics and mechanism. In conclusion, we introduce the concept of a light-dependent activation barrier to account for the effect of light illumination on electronic and thermal excitations in a single unified picture. This framework provides insight into the specific role of hot carriers in plasmon-mediated photochemistry, which is critically important for designing energy-efficient plasmonic photocatalysts.

### **GP-B-03    Toward geometrically guided angiogenesis in 3D printed, perfusable vascularized hydrogels**

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Efforts toward creating functional human tissue mimics must incorporate vascular supplies to sustain viability and maintain functionality of the biological construct. We believe that pre-vascularizing structures with both bottom-up cell self-assembly and top-down bioprinting strategies might enable multiscale, hierarchical vasculature within engineered tissues. We have previously found that human induced pluripotent stem cell derived endothelial cells (hiPS-EC) have an innate capacity to form tubules within fibrin but require co-culture with human mesenchymal stem cells (hMSCs) when encapsulated in gelatin methacrylate (GelMA) to assemble tubules. Pro-angiogenic fibrin provides a well-known standard for vasculogenesis while GelMA possesses photosensitive yet cytocompatible properties for researchers to exploit with photopatterning. We fabricate open vessel architectures in hydrogels with photosensitive materials (GelMA and polyethylene glycol diacrylate) utilizing projection stereolithography. We then endothelialize the channels, forming a monolayer along the interior contours. Using our 3D printing setup, we print acute vascular thorns ( $<60^\circ$ ) and establish fluidic connection through our hydrogels for week long perfusion cultures. We investigate geometrically guided angiogenic sprouting with hiPS-EC lined vessels in response to flow. Our vascular channels incorporate thorn protrusions from which ECs initiate tip cell formation or may migrate as single cells. We determine the extent to which hiPS-ECs sprout from endothelialized channels into the interstitium by measuring sprout length and tip morphology as a result of localized shear stresses and geometric cues. We anticipate that these angiogenic studies, coupled with bulk hydrogel co-culture vasculogenesis, will anastomose to provide vasculature with multi-scale dimensions ranging the span found in native vasculature.

Vascular thorn projections seeded with 10M cells/mL GFP-HUVECs guide angiogenic sprouts after one day of perfusion culture. However in static culture, ECs display a non-continuous monolayer along channel walls. Particle Image Velocimetry allows for tracking of localized velocity vectors in our geometries.



### **GP-B-04 An optoelectronic mid-IR spectrometer**

**Ben Cerjan<sup>1</sup> and Naomi J. Halas<sup>1,2,3,4</sup>**

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Infrared (IR) spectroscopy is a subject of sustained interest in a wide range of fields for its ability to detect and quantify molecules based on their characteristic vibrational resonances. However, traditional IR spectroscopy relies on bulky optics paired with cooled detectors making portability and miniaturization a substantial challenge. In this work we present a demonstration of a room-temperature microscale IR spectrometer and use the device for molecular detection. In addition, this spectrometer was fabricated using only CMOS-compatible materials: aluminum plasmonic gratings on a doped silicon substrate. This work demonstrates a readily scalable approach for fabrication of inexpensive, compact, room-temperature IR spectrometers capable of functioning as a “nanophotonic nose” with direct optoelectronic readout for contact-free molecular detection.

### **GP-B-05 Nucleation and Growth of Aluminum Nanocrystals**

**Benjamin D. Clark,<sup>1,4</sup> Christopher J. DeSantis,<sup>2,4</sup> Gang Wu,<sup>5</sup> David Renard,<sup>1,4</sup> Luca Bursi,<sup>3,4</sup> Runmin Zhang,<sup>3,4</sup> Ah-Lim Tsai,<sup>5</sup> Peter Nordlander,<sup>3,4</sup> and Naomi J. Halas\*<sup>1,2,4</sup>**

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**Abstract:** The precise size- and shape-controlled synthesis of monodisperse Al nanocrystals remains an open challenge, limiting their utility for numerous applications that would take advantage of their size and shape-dependent optical properties. Here we pursue a molecular-level understanding of the nucleation and growth of Al nanocrystals using electron paramagnetic resonance (EPR), nuclear magnetic resonance (NMR) and ultraviolet-visible spectroscopies coupled with transmission electron microscopy (TEM) of the resultant Al nanocrystals. Our analysis indicates low valent Ti ions catalyze reductive elimination of H<sub>2</sub> from aluminum hydride to produce metallic Al, facilitating the formation of Al nanocrystals. The relative rates of nucleation and growth are controlled by the denticity of the solvent ligands, which stabilize Al clusters and nanocrystals through dative bonds. This research establishes a framework for size-controlled synthesis of Al nanocrystals by choice of solvent composition that may enable rational synthesis of shape-controlled Al nanocrystals.

## **GP-B-06 Guiding Protein Conformational Sampling with Experimental Hydrogen Exchange Data to Uncover Unknown Structures**

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A protein's function is known to be modulated by changes in its three-dimensional structure. Interpreting these changes requires gathering information about the protein's conformational space, i.e., the space of all possible protein states. Some information can be obtained experimentally, using techniques such as X-ray crystallography, which has produced numerous structures reported in the Protein Data Bank. To obtain additional information, experimental techniques have been complemented by computational methods such as molecular dynamics. However, experimentally observing and computationally modeling large proteins remain critical challenges for structural biology. Our work aims at addressing these challenges by combining experimental and computational techniques that rely on each other to overcome their respective limitations. Indeed, experimental techniques such as hydrogen-exchange monitoring are increasingly cheaper and easier to implement, but cannot produce structural models because of their low resolution. Therefore, computational methods are needed to complement them and generate structural models. However, these computational methods suffer from the curse of dimensionality when applied to large proteins. To address this issue, a common strategy involves using experimentally-obtained data to guide computational methods. Following this common idea, we have recently proposed a framework in which our own coarse-grained computational method for protein conformational sampling can be guided by experimental hydrogen exchange data. In this poster, we present our latest work; the typical scenario to which it applies is the following: Assuming that an atomistic model of a specific protein state exists, how to obtain a structural description of another protein state for which only hydrogen exchange data is available?

## **GP-B-07 Photothermoelectric detection of individual grain boundaries in microscale gold stripes**

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Nanoscale engineering of thermoelectric properties can be used to enhance performance of photodetection or energy conversion devices. At this scale, the local Seebeck coefficient,  $S$ , can be manipulated by affecting the energy-dependent transport of charge carriers through the material. Simply changing the width of a nanowire causes a change of the electronic mean free path. A width change produces a single metal thermocouple, so that when the interface of the different widths is heated, a measurable open circuit voltage is generated. Even within a polycrystalline gold nanowire of

constant width, substantial local variation of the photothermoelectric voltage is detected due to intrinsic characteristics within the material. To determine the importance of individual grain boundaries to local variation of  $S$ , the spatial photothermoelectric voltages of microscale single-crystal gold stripes with a single grain boundary were measured as a function of a rastering laser used as a local heating source. Surprisingly, both experimental and numerical simulation results show that individual grain boundaries do not act as effective thermocouples themselves, and that other intrinsic factors, such as strain, play a much larger role in the local thermoelectric properties than anticipated. In addition, we note that the grain boundary itself may have its own unique thermoelectric properties compared to the grains themselves.

### **GP-B-08 Crystallographic Selectivity in the Growth of Graphene and Nanotubes**

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Scalable growth of high quality carbon nanomaterials (graphene and nanotubes), seems only possible by precise control of chemical vapor deposition (CVD) conditions. Growth of these materials suffers from issues of polycrystallinity in the case of graphene, and mixed abundance of different chiralities for nanotubes. Synthesis of these materials in their “pure” crystalline phases, has been a longtime goal in the research community. Recent achievements in the growth of large single-crystal graphene films by evolutionary selection mechanism parallels with the experimentally observed high chiral-selectivity of (12,6) nanotubes on solid catalyst, since both lead to selectivity of a specific crystalline phase among several other similar phases.

In this poster, we explain these parallels and their fundamental aspects. First, we explore the concept of “evolutionary selection growth” in the context of 2D materials and how it is the underlying mechanism in the success of growing large monocrystalline graphene by local control of feedstock distribution and no substrate epitaxy. Next, we explain the experimental observations of high abundance of (12,6) tubes for solid Co<sub>7</sub>W<sub>6</sub> catalysts within the framework of our theory of CNT helicity, customized for the specific catalyst facets. We demonstrate using large-scale DFT calculations, that CNT edges prefer to undergo a “phase segregation” and suppress the dependence of the tube interface energy on its chiral angle. Kinetic Monte Carlo simulations were used to study the carbon insertion kinetics, which allowed us to identify conditions that show preference for selectivity of (12,6) tubes.

### **GP-B-09 Near Field Super-Planckian Radiative Heat Transfer**

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**Abstract:** With the advances in nanophotonics and development of new materials, near-field radiative heat transfer has received a renewed interest. Radiative heat transfer between two bodies in the near-field exceeds blackbody limit by orders of magnitude, which stems from the evanescent coupling of the high momentum electromagnetic waves. Here, I present the development of a rigorous simulation framework and set up an experiment to calculate and measure radiative heat transfer in the near-field, respectively. The work also involves exploring potential material systems and investigating their high temperature optical constants. For simulation, I used finite difference time-domain (FDTD) technique based on fluctuation dissipation theorem (FDT) to calculate near-field thermal radiation. The key advantage of this simulation framework is that it can efficiently simulate arbitrary shaped structures and complex material systems. From high temperature optical constant measurement of a test material (GaAs), I show that its optical constant changes significantly with temperature, and thus, need to be considered for accurate simulation and theoretical calculation. Finally, the simple and dynamic nearfield heat transfer experiment, which is based on transient plane source technique, shows that enhanced heat transfer takes place in the near-field regime.



## **GP-B-10 Aluminum Plasmonics at the Single Particle Level**

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Aluminum is a promising candidate for sustainable plasmonics due to its abundance and low cost, and has drawn much attention due to its ability to support high energy UV plasmon resonances. Dark-field spectroscopy is a powerful tool for measuring the scattering response of individual nanoparticles, clarifying their plasmonic behavior. Only recently have synthetic developments allowed study of crystalline nanoparticles. This work demonstrates single particle dark-field characterization of crystalline aluminum particles in the UV and visible regions, accompanied by theoretical calculations to further explore and clarify the plasmonic behavior. Characterization of large Al rods, the first demonstration of such, has determined that rods of varying aspect ratios demonstrate strongly polarization-dependent scattering modes. These are dominated by higher order quadrupolar and octupolar modes across the visible and UV regions, while theoretical calculations additionally predict longitudinal dipoles in the mid and near-IR regions. This work and future characterization of Al nanoparticles expands our understanding of plasmonic Al particles, working towards their application for sustainable, high energy plasmonics.

## **GP-B-11 Toward Single Crystals of Single-Chirality Single-Wall Carbon Nanotubes**

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Carbon nanotubes (CNTs) continue to attract significant interest due to their unique structural, mechanical, thermal, optical, and electrical properties. However, to preserve the extraordinary properties of individual CNTs on a macroscopic level, two challenging goals – alignment and chirality sorting – must be achieved simultaneously. Recently, we have developed a method to fabricate wafer-scale films of highly packed and aligned single-wall carbon nanotubes (SWCNTs), utilizing spontaneous global alignment that occurs during vacuum filtration. Furthermore, by conducting chirality separation prior to the vacuum filtration process, one can use this method to prepare *single-chirality* aligned SWCNT films – a step toward single crystals of SWCNTs. However, perfect alignment (nematic order parameter = 1) has not been achieved for chirality-enriched SWCNTs. To improve the degree of alignment for single-chirality SWCNTs, it is crucial to understand the mechanism of alignment formation during vacuum filtration. Here, we investigated the factors affecting the alignment process and found that the grooves existing on the filter membrane predetermine the direction of alignment. We also applied an electric field during vacuum filtration and studied the interplay of the groove and electric field effects. The application of an AC electric field was found to be able to overcome the groove effect, suggesting that the unique combination of vacuum filtration and electric field application will open the door to the production of large-volume single crystals of single-chirality SWCNTs.

## **GP-B-12 Optical Nonlinearity of 1T-TaS<sub>2</sub> at low intensity and bias tunability of optical properties**

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Transition metal dichalcogenides (TMDs) have been investigated since 1950s. These materials possess many unconventional properties including superconducting, charge density wave (CDW), Weyl semimetal etc., which make them as a potential platform for novel electrooptic devices. In this work, we investigate the optical properties of one of TMDs, 1T-TaS<sub>2</sub>, which performs a phase transition from incommensurate CDW (ICCDW) state to near-commensurate CDW (NCCDW) at 350K, and another phase transition from NCCDW state to commensurate CDW (CCDW) at 180K. We experimentally show that the optical nonlinearity of 1T-TaS<sub>2</sub> happens at low intensity at room temperature. Both reflection and transmission change around 2% at 0.1W/cm<sup>2</sup>. In order to understand this phenomenon, we give an explanation by Hubbard model, in which the electron excited by absorbing a phonon with energy over the hopping barrier can excite the nearby electron and change the optical properties of the system at low intensity of light.

### **GP-B-13 Molecular Nanomachines Kill Bacterial Pathogens**

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Antibiotic resistant pathogenic bacteria are a growing public health and healthcare concern. Several nosocomial infections are multidrug resistant bacteria, and some are “superbugs” that have acquired mutations to develop resistance to commonly used antibiotics. Molecular nanomachines (MNM) consist of light driven synthetic motor chains that revolve at 2-3 million revolutions per second when activated. These MNM, when activated, were recently shown to destroy cancer cells. MNM can have various addend moieties to permit targeting to certain cell types. They can further be designed to have a very fast action rotor or a modification that slows the rotor movement. We exposed fast and slow rotor MNM to three bacteria, *M. smegmatis*, *K. pneumoniae* and *E. coli*, with and without activation. We obtained significant reduction in bacterial viability for each bacterial species. To examine potential toxic effects of MNM on cells, different concentrations of MNM were tested in mitotic mung beans and prostate cancer cells. Studies in proliferating mung beans and *in-vitro* cell culture show that MNM at the concentrations we have used in the cells are not toxic to live cells. These studies provide the proof-of-concept that MNM can be used as an antibacterial agent and that this is due to the nanomechanical action of the fast rotor MNM.

### **GP-B-14 Waste Heat Recovery for Water Treatment: Copper and Carbon**

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Industrial processes often generate large amounts of heat as a byproduct of their operations. This excess heat is wasted energy. Many industrial processes also produce large quantities of contaminated water. This project seeks to capture waste heat with the ultimate goal of treating contaminated water, reducing two waste streams and generating a useful product—clean water. The first stage of this project is examining the utility of copper particles as mid-IR plasmonic absorbers and comparing them to commercially-available carbon black nanoparticles. The copper particles are synthesized in an aqueous

environment to yield a range of particle shapes and sizes, spanning from 500nm to over 5 microns. Both the copper and carbon black have broad-band absorption across the infrared, indicating that they are potential candidates for waste heat recovery. The particles are tested for mid-IR absorption when attached to a porous substrate, polyvinylidene fluoride, to compare the heat absorption properties when secured to a membrane. Future research will involve more detailed comparisons and a combination of chemistry and engineering to build a prototype that absorbs mid-IR radiation and purifies contaminated water.

### **GP-B-15 Understanding protein liquid chromatography through single molecule microscopy**

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Over the past decade, the pharmaceutical industry has moved away from traditional small organic molecules for patient treatment towards protein-based therapeutics, known as biologics. Protein's surface charge, hydrophobicity, and structural dynamics all impose challenges to traditional purification processes. The high cost of protein production can be illustrated by the fact that introduction of each promising biological pharmaceutical to market currently costs ~\$2.6 billion, and half of this cost is the cost of separation and purification. Often proteins surface charge is utilized in ion-exchange chromatography in order to separate proteins from upstream byproducts. Electrostatic interactions of ligand functionalized stationary phase support materials and the target protein are the fundamental driving force of ion-exchange based chromatography. Lysozyme carries a positive charge while Immunoglobulin G is neutral in environments of neutral pH. Lysozyme and Immunoglobulin G were separated using a cation exchange column in a fast protein liquid chromatography system. Single-molecule microscopy was used to quantify protein-stationary phase interaction in real time with high spatiotemporal resolution. A simulation based on the stochastic theory of chromatography developed was used to connect ensemble elutions to single molecule observables. Obtained results provide mechanistic insight into conventional liquid chromatography and allow optimize protein separation.

### **GP-B-16 Width Dependence Study of PL in Gold Nanorods**

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In this research, we systematically investigate on one-photon photoluminescence on three different sizes of gold nanorods. It is well-known that PL of gold nanorods closely resembles their scattering spectra and has two primary features. The main feature in the PL lineshape can be explained using the Purcell effect enhanced hot carrier recombination and the shortband peak in due to interband transitions of gold. In this study, we observe a decrease in PL intensity of the main peak by increasing the size of gold nanorods, which can be explained by quantitatively link Q-factor of the gold nanorods as a resonator and Purcell enhancement effect. However, extra damping in PL intensity is observed for the large sizes of nanorods which cannot be explained only by decreasing of Q-factor. We attribute this extra damping to momentum conservation rules in large sizes where the contribution of intraband transitions is no longer allowed, wherein small sizes due to symmetry breaking intraband transitions are allowed. In our study, we also investigated on the shortband peak in PL spectra of gold nanorods and conducted power and polarization dependence study. Based on our findings shortband peak does not show any size and polarization dependence which indicates even for very large sizes of gold nanorods, where the transverse cross-section is large, we cannot detect any contribution from transverse surface

plasmons in gold nanorods.

### **GP-B-17 Polydopamine Stabilized Aluminum Nanocrystals: Aqueous Stability and Benzo[a]pyrene Detection**

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Aluminum nanoparticles are an inexpensive, sustainable, and powerful alternative to Au/Ag for plasmonic applications, especially in the UV range. However, Al is prone to oxidation in aqueous conditions, limiting its applicability in traditional plasmonic applications. In this work, polydopamine functionalization is adapted to non-aqueous conditions for functionalization of Al nanocrystals, imparting a great degree of new surface chemistry and water stability. Polydopamine coated Al nanocrystals have remarkably long lifetime in aqueous environment, allowing for their implementation as polycyclic aromatic hydrocarbon capture and sensing devices. These harmful organic compounds are sequestered in the polydopamine layer where they can be detected with surface-enhanced Raman spectroscopy. Additionally, these hybrid particles may be capable of contaminant degradation through plasmonic heating or hot electron chemistry.

### **GP-B-18 Increasing yield and long-term stability by using poly(vinylpyrrolidone) during synthesis of gold nanotriangles**

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Gold nanotriangles (AuNTs) are anisotropic nanoparticles that have gained more attention in recent years due to their interesting and unique optical properties that can be tailored for biomedical, energy and sensing applications. At present, few protocols have reported the high yield synthesis of AuNTs of distinct dimensions by the seed-mediated approach. Moreover, there is a need to develop reproducible and scalable methods to aim for the target application. Here, we report an improved seeded protocol for the synthesis of monodisperse AuNTs of different size in high yield with poly(vinylpyrrolidone) (PVP, 10 kDa) as additive. At optimal iodide concentrations, the increment of seed volume produces a blue-shift of the surface plasmon resonance (SPR) band which indicates a reduction in edge length (L) of AuNTs from 75 to 33 nm. It was found that as the edge length decreases, the thickness (T) diminishes from 35 to 20 nm and the aspect ratio (L/T) of AuNTs is modified (2.04-1.64). From the values of extinction coefficient calculated for distinct size of AuNTs, a linear equation is proposed to estimate the concentration of unknown samples by using Beer's Law. Interestingly, the use of nanomolar concentration of PVP during AuNTs growth enhances their shape yield after purification when compared to controls. Based on XPS and ATR analysis, it is suggested that PVP interacts with AuNTs through the oxygen atom of the carbonyl group. Besides, our reproducible and scalable method enables the formation of AuNTs with long-term shape stability (1 year) in aqueous solution.

### **GP-B-19 Vacuum Ultraviolet Light-Generating Metasurface**

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Vacuum ultraviolet (VUV) light has important applications in many fields, ranging from device fabrication to photochemistry, from environmental remediation to microscopy and spectroscopy. Methods to produce coherent VUV light frequently utilize high harmonic generation in media such as rare gases or atomic vapors; nonlinear optical crystals that support second harmonic generation into the VUV are quite rare. Here, we demonstrate an all-dielectric metasurface designed for the nonlinear optical generation of VUV light. Consisting of an array of zinc oxide nanoresonators, the device exhibits a magnetic dipole resonance at a wavelength of 394 nm. When excited with ultrafast laser pulses at this wavelength, the second harmonic at 197 nm is readily generated. Manipulation of the metasurface design enables control over the radiation pattern. This work has the potential to open the door towards simple and compact VUV sources for new applications.

## ***GP-B-20* Ultrafast Electron Dynamics of Single Aluminum Nanostructure**

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Aluminum nanostructures have been a promising alternative material to noble metal nanostructures for several applications, but their ultrafast electron dynamics remain unclear. Here, we combine single-particle transient extinction spectroscopy and parameter-free theoretical calculations to investigate the ultrafast electron dynamics in aluminum nanostructures. Unlike gold nanostructures, the sub-picosecond transient extinction of lithographically fabricated aluminum nanodisks is more sensitive to the lattice temperature instead of electron temperature. We identify a rise, which is independent of pump power, to electron-phonon coupling with a lifetime of about 500 fs. The electron-phonon coupling lifetime is even longer ( $\sim 1$  ps) in aluminum nanocrystals. We also observe a rise and decay whose amplitude scale with the surface-to-volume ratio of the aluminum nanodisks, implying a possible hot electron trapping/de-trapping on the native oxide shell/metal core interface.

## ***GP-B-21* Solving engineering network reliability with quantum spin systems**

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Computing the all-terminal reliability for networks commonly found in engineering applications is of practical importance. However, this problem, denoted  $REL_{AT}$ , is  $\#P$ -hard, that is, the computation time of algorithms that solve this problem scales exponentially with the network size. Recent work has proven that the reliability is exactly upper-bounded by a related Boolean satisfiability counting problem denoted  $SAT_{NET}$ . While  $SAT_{NET}$  is easier than  $REL_{AT}$ , algorithms that solve  $SAT_{NET}$  (such as Monte Carlo, state space partitioning, and statistical learning) also scale exponentially with network size.

To overcome some limitations with the classical algorithms mentioned above, we adapt a quantum algorithm to solve  $SAT_{NET}$ , that for some instances is exponentially faster. Basically, a quantum algorithm is one implemented on machines called “quantum computers” which harness the laws of quantum mechanics at a fundamental level in their information storage and gate operations. In our quantum algorithm, we solve  $SAT_{NET}$  by counting the ground states of a related system of interacting spins on the network, achieved by repeatedly measuring the spins after annealing from a physically easy-to-prepare initial state. Our algorithm can be implemented immediately in several physical experiments on spin systems.

We demonstrate the accuracy and computational efficiency of our quantum algorithm by implementing it on IBM’s “Q Experience” quantum computer for some simple networks. In the future, we will continue to test our algorithm for larger networks, as well as implement our algorithm on other quantum computers such as D-wave.

## **GP-B-22    *In silico* Studies of Aggregation of Amyloid-beta Proteins Using Energy Landscape Theory**

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Although aggregation of Amyloid  $\beta$  ( $A\beta$ ) has received much attention among protein scientists, the question regarding why  $A\beta_{42}$  aggregates faster than  $A\beta_{40}$  is still one major puzzle in the community. Due to the transient nature of  $A\beta$  oligomers and small aggregates, the key to the question apparently lies in the nucleation at the early stages of  $A\beta$  aggregation. We solve this puzzle by exploring and comparing the aggregation free energy landscapes of  $A\beta_{40}$  and  $A\beta_{42}$  which allow us to accurately capture the key molecular event, backtracking, that governs the prefibrillar-to-fibrillar conformational conversion of  $A\beta_{40}$  (which  $A\beta_{42}$  lacks due to the two additional C-terminal residues). Meanwhile, the secondary structure of  $A\beta_{40}$  undergoes an antiparallel-to-parallel conformational conversion. As a result, the backtracking is responsible for slowing the aggregation process. This computational aggregation protocol along with the taxonomy of oligomer clusters that we develop offer a theoretical framework that forms the basis for a library of fully atomistic oligomer structures which may offer specific targets for drug design.

## **GP-B-23    Photocatalytic hydrogenation of graphene on Pd nanocones**

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Photocatalysis utilizes light to drive chemical reactions. Cone-shaped metal nanoparticles possess plasmonic responses when illuminated, with electromagnetic field strongly localized near the tips. When plasmon decays it can generate hot carriers, which can drive chemical reactions near the tip of the nanocones. Here, we show that precisely oriented Palladium nanocones fabricated with nano-lithography can be used as a photocatalyst for hydrogenation of two dimensional (2D) materials, in this case graphene. Graphene flakes synthesized by chemical vapor deposition were transferred on top of Pd nanocones. The plasmonic assisted  $H_2$  dissociation near the interface of the graphene and Pd nanocones generates atomic hydrogen, which turns the graphene into hydrogenated graphene, evidenced by Raman spectroscopy. This model reaction is the first demonstration of photocatalytic chemical doping of graphene, providing a powerful tool for functionalization

and precisely patterning of 2D materials.

## **GP-B-24 Origin of Plasmonic Circular Dichroism from Gold Nanorod-Protein Complexes: A Single-Particle Spectroscopic Study**

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While plasmonic circular dichroism (PCD) has been widely investigated in systems that combine plasmonic nanostructures with chiral biomolecules such as proteins and DNA, a mechanistic understanding of the origin of PCD is often missing in current ensemble PCD measurements. Here we used single-particle circular differential scattering (CDS) spectroscopy to quantitatively investigate the origin of PCD from nanoparticle-protein complexes, in which the Au nanorod-bovine serum albumin (BSA) complex was chosen as a model system. We built a statistical distribution of CDS activity from different nanorod-BSA complexes (single nanorods, dimers, trimers, and more) by taking advantage of single-particle spectroscopy with correlated SEM and TEM images. We demonstrated that single Au nanorod-BSA complexes are CDS inactive, and that Au nanorod dimers, trimers, and larger aggregates complexes show structure-dependent CDS. To gain more quantitative insights into the structure-property relationship, tomographic reconstruction, and FDTD structural simulation are further employed to understand the contribution of chiral structural configuration and chiral protein to the overall CDS. This work provides significant insights into the mechanistic understanding of nanoparticle-biomolecule interactions and the origin of PCD in nanoparticle-protein complexes, as well as potential applications in ultrasensitive biosensing and bioimaging.

## **GP-B-25 Mid-infrared hyperspectral imaging using a quantum cascade laser**

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Hyperspectral imaging is a widely-used method in fields such as astronomy, molecular biology, biomedical imaging and physics for finding objects, identifying materials or detecting processes. Here, we report a new hyperspectral imaging system consisting of a focal plane array detector and a quantum cascade laser. The system allows to map an area  $\sim 200 \times 200 \mu\text{m}^{-2}$  with spatial resolution close to half wavelength and a band width from  $1175 \text{ cm}^{-2}$  to  $1295 \text{ cm}^{-2}$ . To demonstrate its ability to simultaneously measure the spectrum of different structures, a quantitative comparison between the spectrum of bowtie antenna and disk extracted from the same measurement is presented.

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