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Abstracts, Oral Session 1: 9:00 am – 10:30 am

O-1.1 – Photocatalytic Hydrogenation of Monolayer Graphene Using Pd Nanocones

Lin Yuan[1, 5], Chao Zhang[2, 5], Xiang Zhang[3], Minhan Lou[2, 5], Fan Ye[2], Christian R. Jacobson[1,5], Pulickel M. Ajayan[3], Peter Nordlander[4, 5] and Naomi J. Halas[1,2,4,5]
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The interaction between light and metallic nanoparticles can drive chemical reactions on the surfaces of catalysts, a process known as plasmonic photocatalysis. Nanoparticles with sharp tips, nanocones for example, are able to localize the electromagnetic field on their sharp feature (tip of nanocone). Here, we show that a combination of spontaneous H_2 dissociation and hot electron-induced hydrogen desorption from tilted palladium nanocones results in the local hydrogenation of monolayer graphene on top of the nanocones. This is, to our knowledge, the first use of plasmonic photocatalysts to functionalize an adjacent material. The photocatalyzed hydrogenation process transforms monolayer graphene into a semiconductor with a tunable band structure. The conversion can be detected by visible fluorescence of the hydrogenated regions and Raman spectroscopic analysis. These results may lead to new approaches for local, light-driven functionalization of graphene and other two-dimensional materials, as well as precise patterning of functional 2D devices.

O-1.2 – Exploring Size Dependency of Hot Carrier Emission through Interband and Intraband Transitions in Gold Nanorods

Behnaz Ostovar,[1] Yi-Yu Cai,[2] Lawrence J. Tauzin,[2] Arash Ahmadivand,[3]Runmin Zhang,[3]Peter Nordlander,[1,3] and Stephan Link[1,2]
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Light emission from plasmonic nanoparticles has been a matter of focus in recent research because of its possible applications in characterizing hot carriers for selective photocatalysis and photocurrent generation. Inter- and intra-band transitions in gold nanoparticles can generate hot holes and hot electrons, with different efficiency depending on the size of the nanostructure. In this work we quantify the size dependent contribution of interband and intraband transitions to the emission of light from gold nanorods. We use correlated single particle emission and scattering spectra of 120 gold nanorods to calculate their quantum yield and Purcell enhancement factor. We find that in 20-30 nm wide gold nanorods 60-70% of the emission comes from intraband transitions. The efficiency of hot carrier generation through intraband transitions rapidly decreases as the size of the gold nanorods increases to the point that interband transitions become the dominant component. Electromagnetic simulations of the electric field of gold nanorods indicate 2.3 times stronger electric field confinement in smaller gold nanorods providing the necessary momentum mismatch to excite electrons through intraband transitions, in agreement with our experimental observations.

O-1.3 – A mechanistic examination of salting out in protein-polymer membrane interactions

Nicholas A. Moringo[1], Logan D.C. Bishop[1], Hao Shen[4], Anastasiia Misiura[1], Nicole C. Carrejo[1],
Rashad Baiyasi[2], Wenxiao Wang[2], Fan Ye[2], Jacob T. Robinson[2, 3], Christy F. Landes[1, 2]
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Developing a mechanistic understanding of protein dynamics and conformational changes at polymer interfaces is critical for a range of processes including industrial protein separations. Salting out is one example of a procedure that is ubiquitous in protein separations yet is optimized empirically because there is no mechanistic description of the underlying interactions that would allow predictive modeling. Here, we investigate peak narrowing in a model transferrin-nylon system under salting out conditions using a combination of single-molecule tracking and ensemble separations. Distinct surface transport modes and protein conformational changes at the nylon interface are quantified as a function of salt concentration. Single-molecule kinetics relate macroscale improvements in chromatographic peak broadening with microscale distributions of surface interaction mechanisms such as continuous time random walks and simple adsorption-desorption. Monte Carlo simulations underpinned by the stochastic theory of chromatography are performed using kinetic data extracted from single-molecule observations. Simulations agree with experiment, revealing a decrease in peak broadening as the salt concentration increases. The results suggest that chemical modifications to membranes that intrinsically decrease the probability of surface random walks could reduce peak broadening in full scale protein separations. More broadly, this work represents a proof-of-concept for combining single-molecule experiments and a mechanistic theory to improve costly and time-consuming empirical methods of optimization.

O-1.4 – Probing Coherent Terahertz Magnons in $YFeO_3$ in High Magnetic Fields for Ultrafast Antiferromagnetic Spintronics

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There is currently much interest in probing and controlling spin states and dynamics in antiferromagnets (AFMs) for ultrafast information processing. Unlike ferromagnets, for which the speed of spin dynamics is limited to the GHz range, exchange-enhanced spin dynamics in AFMs can be as fast as 10 THz with ultralow power dissipation. Here we study rare-earth orthoferrites, a class of AFMs that exhibit quantum coherent oscillations due to collective spin waves, or magnons, with long coherence times even at room temperature. Due to their canted antiferromagnetic structure, these magnons can be excited by the magnetic-dipolar interaction between the electron spins and the magnetic field component of a THz electromagnetic pulse. We utilize a unique THz time-domain spectroscopy system combined with a 30-T table-top pulsed magnet, which allows us to characterize magnons in orthoferrites in the time domain. Depending on the orientation of the orthoferrite with respect to the polarization of the THz pulse, different magnon modes can be individually excited, or, alternatively, multiple modes can be excited simultaneously and mode-coupling phenomena can be studied. Specifically, we use $YFeO_3$ to characterize coupling between the quasi-ferromagnetic and quasi-antiferromagnetic magnon modes. We successfully excited and characterized these magnon modes and observed resonant coupling in magnetic fields up to 30 T. The resonant mode coupling resulted in an avoided-crossing behavior as a function of magnetic field with a splitting comparable to the resonance frequency, putting the system in the ultrastrong coupling regime, where new phenomena are predicted to occur, including the Dicke superradiant phase transition.

O-1.5 – Convergence of ensemble and single-molecule techniques to understand protein liquid chromatography

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Optimization of protein separation and purification is an empirical process that lacks predictability and is known to be the bottleneck in downstream processing of protein-based drugs. One of the most widely used methods of protein purification and separation is chromatography. However, there is still no detailed molecular-scale picture of protein dynamics during chromatographic separation. The lack of a predictive chromatographic theory is rooted in the absence of an in-depth understanding of interactions occurring inside a chromatographic column. To advance the understanding of underlying phenomena responsible for successful chromatographic separation of proteins, a microscopic, single-molecule picture of the elution process is necessary. The macroscopic picture of chromatography is dictated by processes at the single-molecule level. However, ensemble methods inherently average underlying heterogeneity and, therefore, are not able to yield a full understanding of chromatography on a microscopic level. This work focuses on ion-exchange chromatography (IEX) which separates proteins based on their net surface charge. By using both ensemble and single-molecule techniques we want to develop a mechanistic understanding of IEX. We use Circular Dichroism (CD) to show that negatively charged ligands in cation exchange column cause surface-induced unfolding of the proteins. Using 3D single-molecule fluorescence microscopy we observe increased linear velocities of protein molecules at increased ionic strengths. From our chromatographic profiles, single-molecule results and CD spectra we conclude that lower salt concentrations of a mobile phase lead to stronger surface-induced protein unfolding and lower linear velocity of the protein molecules inside chromatographic column. This work allows us to resolve the details of protein dynamics inside chromatographic column, providing a molecular-scale picture of protein chromatography.

Abstracts, Oral Session 2: 10:45 am – 12:00 pm

O-2.1 – Chemical functionality of Multidomain Peptide Hydrogels governs early host immune responses

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Multidomain Peptide (MDP) hydrogels are nanofibrous materials with potential use in medical and tissue regeneration applications. The design of these materials offers high versatility and allows for the incorporation of diverse chemical functionalities into the scaffold. However, the host response to biomaterials is highly affected by stiffness, size, shape, and chemistry of the materials. Therefore, we evaluated how the peptide sequence design affects the early inflammatory host response to MDP hydrogels displaying various chemical functionalities. The characterization of the immune and inflammatory responses to MDPs was performed using a dorsal subcutaneous injection model. A gross evaluation was achieved by histological analysis, which revealed different degree of cellular infiltration within the implants, as well as blood vessel formation, remodeling rate, and collagen deposition. Further analysis of the cellular infiltrate to each MDP by immunophenotyping in flow cytometry showed different and dynamic cell profiles depending on the chemical functional groups present in the MDP nanofibers. This understanding of the immune response to MDP biomaterials improves our ability to design effective materials for specific applications.

O-2.2 – A copolymer strategy to improve the performance of lithium-ion batteries using polymeric cathodes

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The research on lithium-ion batteries (LIBs) advanced significantly in the past decades. One of the important aspects in the research of LIBs is searching for materials to impart the characteristics of ultrafast-charging and long-term stability to LIBs. Recently, a lot of attention has been paid to semiconducting redox polymers as cathode materials for LIBs because they have proven efficient in transport electrons and lithium-ion (Li^+) storage for their rigid conjugated backbones and redox active structures. Moreover, most semiconducting polymers are solution processable. This research aims to solve a practical problem in the use of semiconducting redox polymers as cathode materials, which is the low Li^+ diffusivity possibly due to the soluble alkyl chains in the polymer structure. A copolymer strategy is introduced to achieve both high electrical conductivity and high ionic conductivity in LIBs through the combination of semiconducting redox polymers with soluble alkyl chains and those with Li^+ transportable polyethylene glycol (peg) chains. This research opens a new avenue in achieving LIBs possessing characteristics of ultrafast charging in a time scale of seconds and long-term stability with thousands of charging-discharging cycles.

O-2.3 – Compressive Microscopy Foveation with the STOne Transform

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Compressive imaging offers the potential to greatly speed up the data-acquisition process for characterizing nanomaterials in various hyperspectral optical microscopies when compared with traditional raster or pushbroom

techniques. However, one of the primary limitations of compressive imaging is the long reconstruction time, especially as the dimensions of the hyperspectral datacube become large. Here we demonstrate a method of decreasing the reconstruction time by foveating over a spatial region of interest determined after the measurements have been acquired anywhere in the field of view. We also present an improved method of computing full-resolution L2-previews that give a higher SSIM relative to a ground truth image than the previous approach. Lastly, we show how our foveation method can be used to parallelize the reconstruction computation to more quickly recover the full-resolution image. Quantitative results are given for both simulated and experimental data, and for grayscale, hyperspectral, and hyperspectral-video data.

O-2.4 – Investigating Cholesterol Orientation in Lipid Bilayer by Raman Spectroscopy

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Gold nanostructures focus light to a molecular length scale at their surface, creating the possibility to determine molecular structures. The high optical intensity leads to surface enhanced Raman scattering (SERS) from nearby molecules. SERS spectra contain information on molecular position and orientation relative to the surface but are difficult to interpret quantitatively. Here we describe a ratiometric analysis that combines SERS and unenhanced Raman spectra with theoretical calculations of the optical field and molecular polarizability. This method can determine specific interfacial structure under ambient conditions, with microscopic quantities of material, and without molecular labels. Previous investigations found that phospholipid bilayers are normal to gold nanorods' surface when they encapsulate the nanorods. While the exact quantity varies by cell type, cholesterol is the next most abundant molecule in cellular membranes behind phospholipids. From molecular dynamics studies, not only do cholesterol molecules interact with the lipid headgroup but also forms pairs and interdigitate within the tail region of the phospholipid bilayer. The results of our structural analysis applied to cholesterol in phospholipid membranes will be presented. Of particular interest is the difference in structure with different quantities of cholesterol, and subtle structural differences among different sterols. Upcoming investigations include examining different anti-inflammatory drugs and different extracellular vesicles.

O-2.5 – Theoretical Investigation of Transcriptional Bursting: a Multi-State Approach

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Variability in gene expression causes genetically identical cells to exhibit different phenotypes. One probable cause of this variability is transcriptional bursting, where the synthesis of RNA molecules randomly alternates with periods of silence in the transfer of genetic information. Yet, the molecular mechanisms behind this variability remain unclear. Experiments indicate that multiple biochemical states might be involved in the production of RNA molecules. Stimulated by these observations, we developed a theoretical framework to investigate the mechanisms of transcriptional bursting. It is based on a multi-state stochastic approach that provides a full quantitative description of the dynamic properties in the system. We found that the degree of stochastic fluctuations during transcription directly correlates with the number of biochemical states. This explains experimentally observed variability and fluctuations in the quantities of the produced RNA molecules. The procedure to estimate the number of relevant biochemical states participating in the transcription is outlined and applied for analysis of experimental results. We also developed a general dynamic phase diagram for the transcription process. The presented theoretical method clarifies physical-chemical aspects of the transcriptional bursting and presents a minimal chemical-kinetic description of the process.

UG-01 – Carbon black-coated membranes for nano-enabled solar membrane distillation (NESMD): A comparison of coating techniques from a scale-up perspective

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Effective water purification methods are crucial for ensuring a stable and safe supply of water to a growing human population on the planet. Solar membrane distillation is one method that can be used to achieve the goal of water purification, and can be augmented by nanotechnology through the use of nanostructured photonic coatings. Several techniques are available to apply such coatings to distillation membranes. However, one must bear in mind that these methods should be easily scaleable, yielding coatings of consistent quality. This study focused on comparing a selection of such techniques to apply nanoparticulate carbon black photonic coatings to polypropylene (PP) mesh support layers as part of a PP-PTFE membrane distillation system. The chosen coating techniques included: dip-coating, drop-casting, spraying, and brush-coating, and incorporated a two-step process wherein a layer of polydopamine (PD) was applied first to provide an interface, followed by a layer of carbon black (the actual nanophotonic material). Each technique has its own pros and cons that will be discussed briefly in this poster, keeping the goal of scaling up the preparation of coated membranes in perspective, through an analysis of observations and data obtained while executing the coating processes. Further work is ongoing in terms of morphological characterization of the coated membranes generated by the selected techniques. This study will help optimize the design and development of nanophotonic coatings for NESMD devices built for scaled-up water purification applications.

Keywords: nanomaterial, photonics, membrane distillation, polymer, carbon

UG-02 – Engineering Thermo- and Photo-Responsive Fluidic Pumps using Liquid Crystal Elastomers

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Liquid crystal elastomers (LCEs) are loosely cross-linked polymer networks with unique optical, mechanical, and physical properties that enable them to shape-shift with thermal stimuli. These unique elastomers have a nematic phase where the liquid crystalline molecules have orientational order at low temperatures and an isotropic phase where there is no order at elevated temperatures. Recent work has demonstrated that dual-network LCEs can be initially cured in the isotropic state, and shape programmed in the nematic state through UV curing. When heated above or cooled below the nematic to isotropic transition temperature, T_{NI}, the LCE can reversibly shape shift between the initially cured and the mechanically programmed shape. Current applications of LCEs range between soft robotics, 4D printing, and biomedical devices. We attempt to expand the potential applications of LCEs by making self-pumping fluidic devices. We program an LCE device to have a collapsible fluidic channel capable of pumping water in response to higher temperatures. In addition, we expand current chemistries to include a photo-responsive dye and additional monomers to produce LCEs with tunable T_{NI} values. The resulting pumps can be controlled using a cascading laser or uniform heat source to yield a bidirectional or one directional pumping, respectively. In the future, the fabrication of these functional LCE fluidic pumps can be translated to a smaller scale in order to create microfluidic devices for alternative applications.

UG-03 – Anomaly Detection for Chatham County Sea Level Sensors

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The Geography of Chatham County, Georgia is nuanced which causes issues in tidal prediction and flood prevention. This motivated the Sea Level Sensors project which aims to create a tide sensor network around the area. Currently monitoring and maintenance of the network is done manually, an approach that is not scalable. This poster details a technique for “anomaly detection” in these sensors. Anomalies are any deviation from the expected water level of a sensor caused by errors with the sensor itself or weather phenomenon. Currently the anomaly detection is used by the Sea Level Sensors project as an email alert system for maintainers as a network and as a data exploration website for the general public.

UG-04 – Anisotropic Magnetic Properties of $Eu(Al_{1-x}Si_x)_4$ Single Crystals

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Single crystals of $Eu(Al_{1-x}Si_x)_4$ were synthesized in order to understand how silicon doping on the aluminum site affects the anisotropic properties. Adding silicon to the body-centered tetragonal $EuAl_4$ leads to a switch from antiferromagnetic order in the parent compound to ferromagnetic order in $Eu(Al_{1-x}Si_x)_4$ when x = 0.25. We map these trends in crystallographic, electronic, and magnetic properties of $Eu(Al_{1-x}Si_x)_4$ in single crystals with x = 0, 0.042, 0.076, 0.113, and 0.139. Here, we report that increases in silicon leads to noticeable changes in unit cell parameters as well as systematic changes in the ordering temperature and magnetic susceptibility anisotropy. Although preliminary data shows that none of the grown crystals order in a simple ferromagnetic ground state, the trend from antiferromagnetic to ferromagnetic order with increasing x is confirmed.

UG-05 – Laser-Induced Graphene Triboelectric Nanogenerators

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Triboelectric nanogenerators (TENGs) show exceptional promise for converting wasted mechanical energy into electrical energy. This study investigates the use of laser-induced graphene (LIG) composites as an exciting class of triboelectric materials in TENGs. Infrared laser irradiation is used to convert the surfaces of the two carbon sources, polyimide (PI) and cork, into LIG. This gives the bilayer composite films the high conductivity associated with LIG and the triboelectric properties of the carbon source. A LIG/PI composite is used to fabricate TENGs based on conductor-to-dielectric and metal-free dielectric-to-dielectric device geometries with open-circuit voltages >3.5 kV and peak power >8 mW. Additionally, a single sheet of PI is converted to a metal-free foldable TENG. The LIG is also embedded within a PDMS matrix to form a single-electrode LIG/PDMS composite TENG. This single-electrode TENG is highly flexible and stretchable and was used to generate power from mechanical contact with skin. The LIG composites present a class of triboelectric materials that can be made from naturally occurring and synthetic carbon sources.

UG-06 – Highly Porous Metal Bio-Polymer Frameworks For Carbon Dioxide Capture

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By virtue of the rapid deprivation of fossil fuels and natural resources, new trends in research activities and the latest technological discoveries have shifted towards effective utilization of a plethora of bio-derived polymers, including animal, agricultural and industrial wastes. To date, several techniques have been revealed to prepare various porous frameworks. However, the possibility of bulk production of these materials requires sophisticated techniques and expensive raw materials which pose a limitation on the scaling-up process. Our proposed project focuses on the development of advanced multifunctional highly porous BioPolymeric Metal Frameworks (BioPolyMFs) materials and a new innovative technology to transform polymeric materials derived from plant and bio-based organic materials. The originality of our proposed work centers in the simplicity, environmental friendliness, and easy availability of the raw precursors and the applicability of the materials towards CO2 capture. The presence of a different range of porosities ranging from submicron to macropores helps in efficient CO2 capture and conversion of trapped CO2 to useful chemicals such as hydrocarbons. This approach helps in environmental degradation substantially and in the discovery of next-generation materials that are optimized for different application such as catalysis, gas absorption, sensors, etc.

UG-07 – A Study of Binders for Graphene-Based Supercapacitors

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Graphene's invention has opened a lot of doors in the field of materials science. Due to its high electronic conductivity and theoretical surface area (2630 m^2/g), it is a very promising material for supercapacitor electrodes with theoretical capacitance of 550F/g. Unfortunately, the re-stacking of graphene layers decreases their electrochemical surface area limiting their use in commercial energy storage devices. Binders used in the electrodes processing play an important role, as they hold the electrode together. In this study, we analyzed the effects of different binders in graphene-based supercapacitor electrodes. The following commercial binders were studied with regards to the graphene electrodes: Carboxymethyl cellulose (CMC), polyvinylidene fluoride (PVDF) and styrene butadiene rubber (SBR). Cyclic voltammetry and impedance spectroscopy coupled with galvanostatic charge-discharge studies are utilized to evaluate the performance of various binders.

UG-08 – Mechanical Exfoliation of Hexagonal Boron Nitride by Ball Milling

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Two-dimensional hexagonal boron nitride (h-BN) sheet can have exotic optoelectrical properties together with extraordinary mechanical robustness, thermal stability and chemical inertness, which are appealing for both fundamental scientific research and commercial applications such as coatings. Compared with other proposed synthesis methods such as chemical vapor deposition (CVD) and liquid exfoliation, ball milling method has the potential to supply a large quantity of high-quality h-BN with reduced thickness. The shearing force during the process can easily break the weak van der Waals interaction between layers and leave the strongly sp2 bonded in-plane structure intact. In this study, an index of the particle size and thickness of h-BN was established after it was ball milled under different conditions: changing the diameter of the grinding media, increasing the ball-milling time, and the mass ratio of ball to h-BN. The

particle size and thickness of h-BN was determined using dynamic light scattering (DLS), scanning electron microscope (SEM), atomic force microscopy (AFM) and x-ray diffraction (XRD). The collected preliminary data can demonstrate the thickness and size of the obtained h-BN under different ball milling conditions.

UG-09 – Comparative Study of Zinc Dendritic Growth on Soft Versus Hard Substrate

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A group of metals including alkali elements and zinc are promising anode materials for the next-generation energy storage systems. The morphological changes of the metal electrodes during charge/discharge is an important factor underlying the stability and performance of metal-based batteries. In particular, the formation of dendritic structure on metal surface during electrodeposition poses a significant challenge because it causes irreversible reduction of battery capacity and even internal shorting of the batteries. Understanding the behavior and the conditions of dendritic growth during electrodeposition is important for the control and suppression of undesirable electroplating morphologies. In this study, we investigate the nucleation and growth kinetics of zinc mossy structure, which is one type of dendritic structure and consists of entangled nanosized filaments. We focus on the effect of plating stress on the mossy growth by comparing the zinc electroplating morphology on hard vs soft substrates. Chemically polished copper foil is used as the hard substrate, and the soft substrate is prepared by sputtering a thin Cu film onto PDMS. Electroplating experiments were systematically performed with varied plating current density and time. The surface morphology of zinc deposits was characterized by scanning electron microscopy (SEM). The obtained SEM images were quantitatively evaluated by image analysis software Fiji to determine the number density and size distribution of zinc mossy clusters. Our analysis shows that mossy zinc has a considerably higher nucleation density on hard than soft substrate, but the type of substrate does not have a significant effect on its growth rate after nucleation.

UG-10 – 3D Printing Liquid Crystal Elastomers to Achieve Direct Shape Programming and Reversible Actuation

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Liquid crystal elastomers are shapeshifting polymers with many potential applications in fields such as soft robotics, artificial muscles, and biomedical devices. LCEs have two states - the nematic, where molecules have orientational order, and the isotropic, where molecules are randomly ordered. The T_{NI} is the nematic to isotropic transition temperature, or the temperature at which the LCE shifts between these two states. Double network LCEs can also be directly programmed into complex shapes by curing the first network in a desired mold, then UV curing it in a desired deformed shape in the nematic state (below the T_{NI}) to complete the second network. As the LCE is heated and cooled it reversibly transitions between the shape during the initial cure and the mechanically deformed shape. While current methods allow for facile synthesis of LCEs that transform between a planar to 3D shape it is more difficult to make LCEs that transverse between two different 3D shapes. Our research attempts to use 3D printing in order to create LCEs that hold complex shapes in both the isotropic and nematic state. The implementation of double network chemistry with an LCE 3D printing method allows for reversible and complex 3D to 3D' shape changes. Future applications include printing a wide range of single and multilayered LCEs, and bi-stable actuation, where it is possible to do large amounts of work at one time, with possible uses in soft robotics and damping structures.

UG-11 – Preparation of Lithium-Ion Batteries Using Redox Conjugated Polymers as Cathodes

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Lithium-ion batteries utilizing redox conjugated polymer as cathodes exhibit fast charging and discharging and excellent stability. Here, we demonstrate how the molecular structure of PNDI-based polymers can be tailored to enhance rate performance and stability. Polymers were synthesized through a Stille polycondensation reaction using a microwave reactor. Half-cell lithium ion batteries were fabricated to test the capacity, rate performance, and stability of organic anodes. Systematic variation of the polymer characteristics (side-chain composition and molecular weights) were studied to understand the impact on performance, and we show that the incorporation of an optimal content of poly(ethylene glycol) (PEG) side-chains produces an optimum in terms of rate capability and stability. This work demonstrates the potential of organic materials for energy storage application where fast charge/discharge is needed.

UG-12 – A Crowdsourcing Approach to Monitoring Freshwater

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Freshwater pollution is a major environmental threat across the globe, exacerbated by the lack of ongoing scientific data about health of freshwater bodies and safety of tap water. One way to address this problem is to crowdsource monitoring of freshwater to citizens. We have developed an integrated mobile phone app which works with a highly cost-effective monitoring kit consisting of chemical test strips. The kit currently measures levels of pH, hardness, alkalinity, total chlorine, free chlorine, copper, nitrates, nitrites, and ammonia using a novel mobile camera-based color detection and contaminant mapping method that avoids human subjectivity in detecting color changes in chemical test strips. The system is designed to be extensible to easily include more parameters. The mobile app geo-tags and uploads all collected data to a global cloud platform that enables interactive monitoring, selection, and visualization of fresh water sources using maps, time periods of interest, or contamination levels. The platform also classifies the overall health of a water source based on its usability for various purposes, compares detected contaminant levels against permissible limits, and generates recommended actions for a polluted water body based on its monitored parameters. An initial pilot with high school students, who monitored ten lakes over several months, shows that this first of a kind end-to-end monitoring system provides new data and insights on changing conditions of freshwater bodies and increases citizen engagement with water issues. We have now refined the system for a larger-scale beta test in the United States and India.

UG-13 – Residue Importance Processing - *In silico* Design of Adeno-associated Viruses to Increase Gene Therapy Vector Transduction Efficiency

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Adeno-associated viruses (AAV) have been proven to be a very promising vector for gene delivery, due to its non-pathogenic, low immunogenic mutagenic properties. It is capable of transducing both dividing and none dividing cells, allowing for broad expression of delivered transgene. Each AAV serotype has a preferential transduction target; specific AAV capsids are selected based on their ability to transduce different tissues. However, it has been shown that there is an increase in neutralizing anti-bodies response as a result of prior exposure to specific AAV serotypes, making repeated dosage of the same AAV serotype ineffective. We seek to recapitulate the different AAV serotypes' ability to transduce specific cells in other AAVs so that we can create AAV variants with similar transduction capabilities while maintaining serotypical diversity. Using machine learning algorithms, we have identified important amino acid residues on the AAV9 capsid that maybe modified to increase its ability to transduce HEK293T cells, which is usually very poorly transduced by AAV9.

UG-14 – Synthesis of Oriented Benzimidazole- and Benzoxazole-Linked Covalent Organic Framework Films

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While there are many theoretical advantages of covalent organic frameworks (COFs) over 1D polymers, COF synthesis typically yields an insoluble powder, which is incompatible with various applications such as mechanical testing and integration into electronic devices. Drawing inspiration from the structures of rigid one-dimensional (1D) polymers like polybenzimidazole (PBI) and polybenzoxazoles (Zylon), some of the highest strength and thermally-resistant materials to date, we have successfully designed a novel method for producing films of 2D COFs with benzimidazole and benzoxazole linkages. These films are synthesized via a simple solvothermal method, where the precursor solution is drop-casted onto glass substrates and heated to initialize the formation of dynamic bonds between monomers, creating a pre-polymer film. These intermediate films are then annealed under vacuum to convert the dynamic linkages irreversibly to the final product. Varying the volume and concentration of the precursor solution allows for modulation of film thickness from 3 μm down to about 60 nm. Thus far, crystalline film samples of both the benzoxazole and benzimidazole structures have been obtained. The two-step process enables highly crystalline films as the COF molecules orient during the solvothermal step due to the hydrogen bonding between intermediates and are further crystallized during annealing. Finally, mechanical testing was performed on the free-standing benzoxazole COF films, obtaining an ultimate tensile stress and Young's modulus comparable to commercial 1D polymers. Future work will focus on expanding the library of high strength linkers and improving crystallinity of the resulting films to better study the intrinsic properties of these materials.

UG-15 – Analyzing Properties of Concrete with Embedded Plastic/Foam

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The objective of this project is to determine the properties of concrete with embedded plastic bottles and foam to better understand the performance of sustainably built structures using these materials. The use of these materials in building is fueled by the desire to reduce building costs and to keep plastics and foam out of the landfill. The samples consist of concrete and different arrangements of the embedded materials. Each sample is 3 ½" x 2 ¼" x 8" to allow an entire plastic bottle to be embedded in the sample. Samples contain 1) different sizes/shapes of bottles, 2) bottles with additional filling (plastic/foam), 3) large pieces of foam, and 4) foam/concrete mixture. The samples are tested for thermal properties, water resistance, and loading. The results from this analysis will benefit those seeking to build low cost sustainable structures while understanding the behavior of the material under various conditions around the world.

UG-16 – Educational Brain CAD Model

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In this research project object, our aim was to create and print the brain model into 8 educational section aided computer-aided design (CAD). Since a suitable AutoCAD model is not available and the price of the commercially available model is over $500 which surpassed our cost. The project started within the Honor of Engineering Graphics classes in which we would split the brain into 6 different groups made up of 2 people, which were assigned different parts. Our team was assigned the brain stem which includes the midbrain, the pons and medulla oblongata of the hindbrain. Overall this project was composed of 4 phases 1)research the brain stem to be able to recreate it with as much detail as possible, 2)research on various CAD programs to determine which would be able to create the brain model, 3)design our assigned part using the CAD program with a good amount of detail and communication with our peers ,4) printing and fitting all sections together During the first phase, we attended a class to observe a sheep brain dissection, examined it and their brain models while work with the biology department on how to improve the brain models in more features. The second phase was trying to discover the type of program to utilizes to perform the design which includes AutoCAD, Solid works, Blender, Rhinoceros, Qlone, and Sculptris. During the third phase, we had a collaboration where we used Qlone to scan the model for size and shape, and blender and AutoCAD to create all specific features to improve it. So, by phase 4 all the groups have finished their assigned parts, where we successfully made a complete the model for the brain. The final brain met the initial requirement and the final cost $20 per model to print.

NANO-01 – Single-Particle Optical Spectroscopy to Monitor Copper Nanoparticle Rate of Change

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Selective reduction of carbon dioxide into more efficient carbon-based products (e.g. ethylene, ethanol, n-propanol) creates the possibility for different fuel resources and fuel precursors. Copper nanoparticles have been shown to efficiently catalyze these carbon dioxide reduction reactions with negative potentials. Throughout the electrocatalytic reduction reaction, the copper nanoparticles structurally transform into cube-like structures, however imaging via electron microscopy is only possible before and after the reaction. To address the knowledge gap regarding this kinetic rate of nanoparticle transformation, in situ single-particle scattering microscopy is proposed as copper nanoparticles have localized surface plasmon resonance (LSPR). A transparent working electrode is necessary for such microscopy and currently used indium tin oxide is unstable at the negative potentials needed to catalyze the carbon dioxide reduction reaction. This project tests different conductive transparent surface coatings on soda-lime-silica glass to improve electrode performance. By utilizing thin film deposition techniques, gold substrates were created for the deposition of copper nanoparticles. The synthesis of copper nanoparticles into nanocubes was successful as confirmed on a scanning electron microscope. However, the LSPR of the synthesized copper nanoparticles requires confirmation on a UV-Visible Spectrophotometer. Differentiation of signal between the nanoparticles against gold is currently being tested, as the signal-to-noise ratio must be determined before concluding if the gold thin film is a viable solution. Success in this project will provide a unique perspective on understanding electrocatalysis, allowing proper modeling of complex data for the chemical engineering field.

NANO-02 – Temperature Analysis at a Molecular Scale

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Cell membranes regulate what can enter the cell through delicate molecular interactions that are affected by the fluidity and permeability of the cell wall. We will study the fluidity of lipid bilayers, a model for biomembranes, because it is strongly affected by temperature. Surface enhanced Raman scattering via Raman spectroscopy will be utilized for temperature determination at a molecular scale. As the lipids give a weak Raman scattering signal by themselves, the lipid bilayer will be added to gold nanorods (AuNR) to enhance the signal via plasmon resonance. The Raman Scattering yields stokes and anti-stokes spectra that will be analyzed in order to obtain molecule-specific vibrational peaks in the Raman spectrum. These will be inserted into a formula that will yield the absolute temperature. Preliminary tests were performed at room temperature to establish a method of executing temperature analysis effectively. These preliminary tests involved the use of solid polytetrafluoroethylene (Teflon) and AuNRs suspended in Cetyltrimethylammonium bromide as these provide strong peaks. The temperature obtained from the Teflon experiment has been relatively precise as temperature measurements on different peaks vary by only 10K and were close to room temperature at an averaged 282K. Once temperature analysis with lipids placed on AuNRs are performed, the data derived from their related peaks will demonstrate if the absolute temperature can be deduced. This can lead to the further understanding of cell membranes and the possibility of making medical and chemotherapeutic agents more effective as they interact heavily with the cell membrane.

NANO-03 – Shear Coupled Grain Boundary Migration

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We present a new tricrystal growth technique and the consequent observation of shear coupled grain boundary movement in tin tricrystals. These particular tricrystals are grown using 3D printing crystal growth technique which fabricates large scale crystals with controlled microstructures. The samples are then cut and polished and tested for grain boundaries under a microscope. They are finally annealed (slow heating) in a controlled and isolated environment where driving forces acting on the grain boundary tend to cause grain boundary motion and grain rotation. The observation of such motion is examined using microscopy, where the entire annealing process is recorded under a microscope and pre-and post-annealed sample pictures are compared. The grain boundary migration rates are eventually calculated using image/video processing.

NANO-04 – Laser-Induced Graphene for Air Filtration

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Modern day hospitals are plagued by Healthcare Associated Infections (HAI) which may be diminished by air filtration. According to the Centers for Disease Control website, the probability of a U.S. patient contracting at least one HAI during hospitalization is 1 out of 31. Approximately 10-20% of HAIs are spread by airborne mechanisms. Joule heated Laser-Induced Graphene (LIG) filters have been demonstrated to effectively capture and incinerate airborne pathogens. This work demonstrates the ability of LIG filters at removing and incinerating airborne particulates that carbonize around 300°C to 350°C, thus preventing filter clogging. To simulate a rapid aging process, airborne particulates are agitated onto the LIG filter while monitoring filter clogging by measuring the pressure drop across the filter. A voltage was applied to the filter to Joule heat and incinerate the entrapped material. It was demonstrated that LIG filters will partially recover the initial pressure drop associated with an unclogged filter after accelerated aging followed by Joule heating. The airborne particulates under test, in some cases, had components that would not decompose by carbonization, for example: silica and glass. LIG filters successfully unclog by incinerating entrapped organic particulates, as seen with bee pollen, in which the filter pressure drop recovered approximately 80% after Joule heating the filter.

NANO-05 – 3D printing under visible light using cadmium selenide semiconducting quantum dots as photoinitiators

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The development of 3D printing, also known as additive manufacturing, has allowed the fabrication of complex objects with a widespread application in various fields such as medicine and engineering. Photopolymerization, one of the most attractive 3D printing approaches, utilizes photoinitiators that initiate the reaction under light absorption. The photoinitiators used so far for 3D printing suffer from high catalyst loading and inhibition in the presence of oxygen. In this work we report a new photoinitiating system consisting of cadmium selenide semiconducting quantum dots (CdSe QDs) as photoinitiators and 3-Mercaptopropionic acid (MPA) as co-initiator to achieve gelation of poly(ethylene glycol) diacrylate (PEGDA) under the irradiation of blue light. By only using ppm levels of CdSe QDs, it is possible to achieve good resolution 3D printing process using digital light processing (DLP) 3D printer. The excellent performance of CdSe QDs/MPA initiating system in 3D printing photocurable material PEGDA opens up great opportunities for fabricating widespread polymeric materials via 3D photoprinting process.

NANO-06 – Size-dependent interfacial tension and phase equilibrium of paramagnetic colloidal clusters under a time-varying magnetic field.

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Late advancements in chemistry, physics, materials science and nanotechnology have allowed the synthesis of new materials with enhanced properties and improved efficiency. Despite this, complex phase transformations and behaviors preclude the development and further applications of these technologies by decreasing the effectiveness of their performance. To further study such processes in-depth, we propose a model based on the dynamics of paramagnetic colloidal systems in resemblance to molecular self-arrangements and interactions. Colloids are highly dynamic structures that rely on thresholds of energy to undergo phase transitions. Moreover, superparamagnetic colloids allow an external magnetic field to act as an apparent temperature of the system, under which an initially homogeneous suspension can exhibit properties specific to crystallites or liquid droplets, depending on the strength of the magnetic field. In the following study, we characterize the interfacial stiffness of colloidal aggregates in relation to size by exposing suspended samples of carboxyl-coated particles to high-frequency magnetic fields of different strengths. Upon analysis, we have observed a decline in interfacial tension reciprocal to cluster size. These results are coherent with Richard Tolman's equation of surface tension vs. droplet size, which predicts similar behavior in nanodroplets of molecular diameter. Furthermore, we demonstrated how cluster equilibrium in its homogeneous phase entails to the manifestation of vapor pressure and its relation to cluster size in an isolated system. For future experiments, we propose a supplementary analysis of the physical properties of paramagnetic colloids for the understanding and development of a predictive model of molecular behavior.

RSTEM Research Experience for Undergraduate (NEWT) Poster Session Abstracts

NEWT-01 – Engineering safe carbon nanomaterials: role of morphology and surface chemistry in the interactions of carbon nanomaterials with microorganisms

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Carbon Nanomaterials (CNM) are significant because they are used in healthcare to improve dental implants, in electronics to better capacitors, and to improve water treatment technologies. CNMs such as carbon nanotubes (CNTs) and graphene oxide (GO) are significantly being produced more than ever before, but there has not been enough research regarding the proper design criteria needed to achieve a safe use of carbon-based nanotechnologies through the fabrication of benign CNMs. This project focuses on the effect of surface chemistry on the interactions of GO and CNTs with *Scenedesmus obliquus*, a green algae primarily found in freshwater. A dose-response was done using concentrations from 0 to 100 µg/mL of CNM. Results indicate that at 73 and 48 µg/mL, CNTs and both the thermally annealed CNT400 and CNT600 reduce chlorophyll content by 50% (EC50), respectively. Chlorophyll *a* decreased significantly starting at CNT400 concentrations of 10 µg/mL and 25 µg/mL for CNTs and CNT600 with respect to control after 24h of exposure. On the other hand, GO showed no chlorophyll inhibition at the tested concentrations. These results were compared with previous hazard characterization using the gram negative bacteria *Escherichia coli*. The green alga is found to be less sensitive than bacteria to the effects of CNM. These results provide useful insights into the effect of surface chemistry on the toxicity of different carbon nanostructure, GO and CNTs, which will allow for a safe design of carbon-based nanotechnologies.

NEWT-02 – Membrane Distillation of Produced Water from the Oil and Gas Industry: The Effect of Membrane Fouling using a Bench-Scale Solar and Conventional Membrane Distillation System

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Produced water, or oilfield brine, is generated during processes related to the hydraulic fracturing and refining of oil that is extracted from natural geologic reservoirs. Currently, the volume of this hazardous, high salinity, wastewater exceeds the output volume of produced oil. In order to minimize the discharge of wastes into the environment and avoid the exhaustion of valuable water resources, water management strategies to recycle and re-use produced water, a notion known as zero liquid discharge, are being investigated and implemented. Conventional membrane distillation is a thermal-driven, vaporization-based, water purification technology that is ideal for removing both the inorganic and organic dissolved particles inherent in produced water. Nanophotonic-enabled Solar Membrane Distillation is a novel technology developed at the Nanosystems Engineering Research Center for Nanotechnology-enabled Water Treatment (NEWT) at Rice University that utilizes solar thermal energy to heat and vaporize water, thus lowering the energy requirements relative to conventional membrane distillation. Although both systems are efficient in desalinating wastewater, the possibility of enhancing cost- and energy-efficiency, as seen in Solar Membrane Distillation, is promising. This study examined the effect of produced water on the fouling of both solar and conventional membranes using a bench-scale membrane distillation system. The membranes were characterized in terms of their hydrophobicity, pore size distribution, and performance before and after the treatment of contaminated waters obtained from two different sources. Membrane characterization was then related to the chemistry of the treated water in terms of conductivity, total dissolved solids, pH, total organic carbon, and turbidity.

NEWT-03 – Field Demonstration of Nanophotonics-Enabled Solar Membrane Distillation (NESMD) for Desalination

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Nanophotonics-enabled solar membrane distillation (NESMD) is a highly innovative off-grid, chemical free technology that can take almost any source of water and turn it into potable water with sunlight as the only energy source. NESMD simultaneously achieves solar thermal energy harvesting and desalination using a photothermal membrane in a single reactor. Research and developments have been done to the NESMD reactor using different sources of water with varying total dissolved solids (TDS), including RO concentrate (17,000 ppm), Galveston sea water (20,000 – 40,000) and simulated water (20,000 - 200,000). A 99.5% TDS removal has been achieved, for all water sources, under various environmental conditions. Also, a permeate flux of 0.7 L/m^{2}hr. and higher was achieved at solar irradiation of 1000 W/m^2. To keep the NESMD reactor from fouling, deionized water was run through the reactor after every test, in a process called forward washing. To increase efficiency in terms of amount of water produced, a unique multi-lensed system has been designed, developed, and tested. Although in its early stages, NESMD is a promising advancement that could lead to an innovative and environmentally friendly alternative to current water treatment technologies.

NEWT-04 – Capturing Water Out of Air: Solar-Light Activated Photothermal Nanomaterial Enabled Desiccants Improve Water Vapor Desorption Efficiency

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During a natural disaster such as earthquakes, floods and/or droughts clean water can be scarce and is generally provided by distributing bottled water or membrane filtration. These approaches can be costly, and wasteful. Atmospheric water capture (AWC) devices can be used in these situations to recover water directly from the atmosphere. In AWC, water is adsorbed from the atmosphere and into a desiccant. The desiccant is heated to release water vapor, which is then condensed into potable water. This heating process is energy intensive, but we can create an off-grid solution if we use photothermal nanomaterial enabled desiccants (PNED). These enabled desiccants use naturally occurring sunlight to superheat the desiccant eliminating the energy cost. To quantify the benefits of PNEDs, the desiccant SiO_2 was coated in gold nano rods, gold nanocubes or carbon black, and each was individually tested for increased water desorption. We hypothesize that carbon black-coated desiccants will heat fastest and desorb water vapor fastest because they absorb light in the entire solar spectrum.

NEWT-05 – Efficacy and Characterization of Layered Double Hydroxide-Chitosan Nanocomposite Beads for the Selective Removal of Selenium Oxoanions from Water

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Selenium is an essential micronutrient that promotes regular cell growth and development but can be toxic to humans and wildlife in concentrations of 2-5 µg/L and is commonly found in industrial wastewater and agricultural runoff. Due to their similar molecular structures, sulfate adsorption competes with selenate, reducing the efficiency of water treatment. Mg-Al-CO_3 layered double hydroxide (LDH) nanoparticles embedded in chitosan nanocomposite beads are effective sorbents for the removal of selenate from water. To improve the selectivity of LDH sorbents for selenate over sulfate, a molecular imprinting approach was investigated in this study. Templated LDH beads are formed by first introducing the LDH powder into a selenate spiked solution, to adsorb the selenium into the interlayer of the compound. After incorporation of the LDH into the chitosan, the selenium is desorbed to create selective cavities as binding sites. Non-templated LDH beads are formed by placing the pristine LDH powder directly into the chitosan polymer. We evaluated the efficacy of templated and non-templated LDH-chitosan beads to selectively remove selenium from water in jar tests. Solutions with selenium to sulfate ratios 1:0, 1:1, 1:10, and 1:100 were tested, and selenium concentrations were quantified before and after the tests using inductively coupled plasma mass spectrometry (ICP-MS). The composition of the synthesized nanocomposite materials was confirmed using Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and x-ray diffraction (XRD). The ICP-MS results show that the removal rate for selenate and sulfate is higher in templated LDH compared to non-templated LDH.

NEWT-06 – Synthesis and Characterization of FeOOH and AlOOH for the Selective Removal of Selenate in Simulated Drinking Water

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Selenium is an inorganic water contaminant which exists as an oxyanion in multiple oxidation states, prevalently as selenite (SeO_3^{-2}) and selenate (SeO_4^{-2}). Selenate is known to be more toxic, bioavailable and mobile than the reduced form, selenite. However, its removal from water is hindered by isostructural oxyanions (such as sulfates and phosphates) which are present in large quantities in water. Previous work has demonstrated that different crystal facets of hematite preferentially promote the adsorption of selenate over selenite. In order to further probe the crystal facet-selectivity relationship, the present work compares the selenate adsorption capacity of iron and aluminum oxyhydroxides. Goethite and boehmite (α-FeOOH and γ-AlOOH, respectively) samples were synthesized and characterized through pXRD, TEM and BET in order to confirm their crystallinity, crystal shape and surface area. Selenate adsorption experiments for both samples were performed in a simulated drinking water matrix in order to mimic realistic conditions and probe their selenate adsorption capacity in the presence of competing ions. Adsorption results were fitted into a Freundlich adsorption isotherm in order to obtain the maximum adsorption capacity of both materials. Further work involves the crystal facet identification of the prepared samples through high resolution transmission electron microscopy (HR-TEM) along with the repetition of the adsorption experiments using lepidocrocite (γ-FeOOH), diaspore (α-AlOOH), and amorphous $Al(OH)_3$.

NEWT-07 – Categorizing Ion Excluding Membrane Efficiency for Electrodialysis

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Electrodialysis (ED) is the process of using an electric field and ion-selective membranes to separate and concentrate ions. Anion Exchange Membranes (AEM) and Cation Exchange Membranes (CEM) are the two main types of membranes used. Many different types of AEMs and CEMs are available in the market, each with their own advantages and disadvantages. The effectiveness of a membrane is dependent on many factors, including the ion concentration in the water being treated, the voltage applied to the ED stack, and the flow of water through the stack. For this study, combinations of five ion concentrations, three voltages, and three flows were tested on fifteen commercially available membranes. The ED trials are run for one hour each, conductivity values are measured throughout at five second intervals. Conductivity is then used to compare the effectiveness of each membrane. The performance data will be compiled and organized in a database that will be useful for ED users to select the membrane type most suitable to their needs.

NEWT-08 – Transition Metal Nanoparticles Embedded on Porous Carbon Matrix for Environmental Remediation

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Organic pollutants in water are difficult to remove and dangerous to the public and environmental health. The presence of textile dye in water is deleterious towards the public as well as aquatic life. Transition metal nanoparticles (Cu, Ni, Fe, Co) embedded on porous carbon were prepared by carbonizing the metal organic framework and used as a Fenton-like catalyst to remove organic pollutants from water. The as-prepared nano-catalysts were characterized using SEM, EDS, TEM, FT-IR, XRD, TGA and BET. XRD analysis confirmed the pure metallic face of all the nano-catalysts. TEM analysis revealed that all the metal nanoparticles were encapsulated on the porous carbon matrix. Catalytic studies suggested that the nano-catalysts were highly catalytically active, stable and reusable. For the catalytic experiments, several factors such as initial dye concentration, oxidant (peroxymonosulfate, dioxymonosulfate and H2O2), temperature, and different types of dyes were studied. Their catalytic activity followed the order Co > Fe > Cu > Ni in the presence of peroxymonosulfate. Additionally, quenching experiments revealed that the sulfate is a radically dominant species in the dye degradation process. In conclusion, these results provided enough evidence to demonstrate the effectiveness of transition metal nanoparticles in the removal of organic pollutants from water.

Abstracts, Oral Session 3: 2:00 pm – 3:15 pm

O-3.1 – Engineering mind-reading biosensors: High-throughput development of voltage indicators for *in vivo* neuroimaging

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A longstanding goal in neuroscience is to understand how spatiotemporal patterns of neuronal electrical activity underlie brain functions. An emerging technology for real-time monitoring of electrical dynamics *in vivo* is voltage imaging using Genetically Encoded Voltage Indicators (GEVIs) — engineered light-emitting protein indicators whose brightness directly reports voltage. Despite significant progress made by the GEVI community so far, the performance of current voltage indicators still needs further optimization to allow long-term deep-tissue imaging of many individual neurons in behaving rodents. Here we present an automated platform for high-throughput screening of GEVIs libraries using field stimulation of mammalian cells, followed by detailed characterization of the most promising candidate identified during our screens of libraries based on the Accelerated Sensor of Action Potential (ASAP) family indicator, which are now referred as Jellyfish-derived Electricity-reporting Voltage Indicators (JEDIs). We anticipate that these efforts will ultimately produce high-performing indicators of broad utility for imaging spontaneous voltage dynamics in the brains of behaving animals.

O-3.2 – Optical modulation of optical properties of 1T-TaS$_2$ at low intensity

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Transition metal dichalcogenides (TMDs) have been investigated since 1950s. These materials possess many unconventional properties including quantum spin liquid, 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$_2$, 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$_2$ happens at low intensity at room temperature. Both reflection and transmission change around 4% at 0.1W/cm^2, indicating a large tunabilities of refractive index around 0.4 in visible. We also demonstrate that such photo-refractive effect of 1T-TaS$_2$ exhibits a response speed to light excitation higher than 100 kHz, which probably is due to thermotical effect. At the end, we implement the tunable refractive index of 1T-TaS$_2$ to make a meta-grating device and experimentally demonstrate 0.3 degrees change at 540 nm under different light excitations.

O-3.3 – In situ detection of plasmonic nanoparticle transformation during catalysis on the single particle level

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Syngas and formic acid production by the electrocatalyzed CO$_2$ reduction reaction are economically viable;

however, products with two or three carbons have yet to be realized. Plasmonic copper nanoparticles on glassy carbon show promise and have out-performed copper films as electrocatalysts for the production of C_2-C_3 products, but ex situ electron microscopy revealed the nanoparticles had transformed to new sizes (7 nm or 52 nm to 24 nm) and shapes (hexagons to cubes). Currently, electron microscopy cannot track an aqueous, gas-forming reaction in situ. Opportunely, a plasmonic metal nanoparticle scattering spectrum is highly susceptible to changes in surface structure and size, well tracked with single-particle darkfield scattering microscopy. A model gold nanorod surface was studied undergoing reduction with $NaBH_4$, to confirm the assumption that morphological changes can be detected during gaseous product formation. This presentation discusses the microscope built to detect dissolution-redeposition in situ and the role of nanoparticle shape and size dependence on the blue shift of scattering wavelength. 1 ms resolution and a flow-through geometry to replenish reactants and transport gas was achieved. Furthermore, gold nanorods were confirmed to be an ideal model to test the microscope's ability to resolve nanoparticle transformations during gas forming reactions. Single particle microscopy can track the kinetics of in situ nanoparticle structural transformations. This in situ method will give time resolved tracking to determine the morphological dependence of nanoparticle shape changes that occur within an electrochemical cell. It is crucial to understand crystal transformation mechanisms to design more efficient electrocatalysts.

O-3.4 – Hot Start Formation Implied by Detection of CO in CI Tau b

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We acquired high resolution IR spectra of CI Tau, the host star of one of the few young planet candidates amenable to direct spectroscopic detection. We confirm the planet's existence with a direct detection of CO in the planet's atmosphere. We also calculate a mass of 11.6 M$_J$ based on the amplitude of its radial velocity variations. We estimate its flux contrast with its host star to get an absolute magnitude estimate for the planet of 8.17 in the K band. This magnitude implies the planet formed via a "hot start" formation mechanism. This makes CI Tau b the youngest confirmed exoplanet as well as the first exoplanet around a T Tauri star with a directly determined, model-independent, dynamical mass.

O-3.5 – Resonant Heat Transfer for Solar Thermal Desalination

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Water scarcity currently affects 40% of the global population and is one of the most significant challenges of the 21st century. As the world population, industrialization and climate change effects grow, water scarcity is becoming an increasing concern. Meeting the demand for fresh water requires new innovative water purification technologies to exploit the alternative saline, processed, or brackish water sources. Evaporation based thermal distillation is effective and essential to treat such high-salinity water reservoirs, but the phase change process is intrinsically energy intensive, necessitating alternative energy sources such as solar power. One major challenge for solar-based desalination is increasing the process efficiency with cost-effective techniques to achieve sufficient fresh water production capacities at less than 1 Sun. In this work, we obtain a thermal efficiency of ~150% with a fresh water flux of ~1.1 L/(m$^{2}\cdot$h) under 0.475 Suns. Our approach combines a nanophotonics-enabled solar membrane distillation (NESMD) system with a dynamic thermal recovery mechanism. By optimizing the flow rates of the water, thermal energy in the system is efficiently recycled as in an oscillator. We numerically predict water production of 20.5 L/m^{2} for an optimized system during a typical sunny day. The resonant heat recovery approach is general and can be applied to any open photo-thermo-fluid-dynamic systems like thermal energy storage and solar powered chemical reactions.

Abstracts, Oral Session 4: 3:30 pm – 4:45 pm

O-4.1 – Methane Bioreforming for the Production of Ammonia: A Microbial Consortia “Bio Haber-Bosch”

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Plants require nitrogen for protein biosynthesis and growth, but fixed, usable, nitrogen (NH_3, NO_3, urea) is a naturally limited resource that is typically supplemented as fertilizer to achieve modern food crop yields. Today, nitrogen fertilizers feed one in two global citizens, but access to fertilizers remains a barrier to increased crop yield globally. While the traditional chemical industry can efficiently produce fixed nitrogen products such as ammonia (NH_3) at large scale, the required high temperatures and pressures (450°C, 200 atm) limit the transferability of Haber-Bosch technology to use of low-volume and remote waste methane (CH_4) feedstocks that were recently identified to exist on a global scale. With unequal global fixed nitrogen distribution and overall foodstuffs demand anticipated to increase during the next century, the development of alternative methods for ammonia (NH_3) synthesis and small-scale methane (CH_4) energy capture that operate at ambient temperatures and pressures (30°C, 1 atm) is highly desirable and motivated development of a biomanufacturing process with joint CH_4 and nitrogen gas (N_2)-in-air feedstocks for bioproduction of NH_3. The system contains a microbial consortium of *Azotobacter vinelandii* M5I3 and *Methylomicrobium buryatense* 5GB1 pAMR4-dtom1 performing methane bioreforming (MBR) and biological nitrogen fixation (BNF). Proof-of-concept experiments were carried out to identify the fate of carbon and nitrogen products in the system and optimize co-culture growth conditions. This contribution discusses development of the ambient CH_4-driven NH_3 biosynthesis system, the products of which could be either recovered for direct external application or utilized as a tool to drive higher-value bio-product formation.

O-4.2 – Aluminum Nanocubes have Sharp Corners

Benjamin D. Clark,[1,4] Christian R. Jacobson,[1,4] Minhan Lou,[2,3] David Renard,[1,4] Gang Wu,[5] Luca Bursi,[2,4] Arzeena S. Ali,[1,4] Dayne F. Swearer,[1,4] Ah-Lim Tsai,[5] Peter Nordlander,[2,3,4] and Naomi J. Halas[1,2,3,4]
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Of the many plasmonic nanoparticle geometries that have been synthesized, nanocubes have been of particular interest for creating nanocavities, facilitating plasmon coupling, and enhancing phenomena dependent upon local electromagnetic fields. Here we report the straightforward colloidal synthesis of single-crystalline {100} terminated Al nanocubes by decomposing AlH_3 with Tebbe’s reagent in tetrahydrofuran. The size and shape of the Al nanocubes is controlled by the reaction time and the ratio of AlH_3 to Tebbe’s reagent, which, together with reaction temperature, establish kinetic control over Al nanocube growth. Al nanocubes possess strong localized field enhancements at their sharp corners and resonances highly amenable to coupling with metallic substrates. Their native oxide surface renders them remarkably air-stable. Chemically synthesized Al nanocubes provide an earth-abundant alternative to noble metal nanocubes for plasmonics and nanophotonics applications.

O-4.3 – Measurement of 3-body losses in a quasi-1D ^{6}Li gas near a *p*-wave Feshbach resonance

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P-wave interactions are known to lead to phenomena such as p + ip superfluids and Majorana fermions. These phenomena exhibit intriguing topological behaviors that are relevant for new approaches in quantum computation. However, the three-body recombination collisions that occur near a p-wave Feshbach resonance result in severe atom losses, and thus the experimental detection of these phenomena in 3D ultracold atomic gases remains a challenge. Recent theoretical predictions suggest that such effects could be suppressed in low-dimensional confinements, thus leading to the formation of p-wave atom pairs un such regimes. To study the stability of these pairs, we measure the three-body loss rate using ^{6}Li atoms that are spin-polarized in the Zeeman ground state $|f = 1/2, m_f = 1/2>$. The atoms are subjected to a quasi-1D confinement by using a 2D compensated optical lattice. We report the result of the three-body loss rate measurement in different dimensions.

O-4.4 – Modularity and Flexibility Quantify Unique Perceptions of Music and Speech in the Human Brain

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Music therapy is effective for improving cognitive health in patients suffering from neurological disease or trauma, however little is known about the mechanism of action and lacking are studies that quantify the impact of music on the brain. Modularity and flexibility are two quantifiers of functional brain activity that have been demonstrated to predict the relative performance of subjects on cognitive tasks of varying complexities (Yue 2017, J Cogn Neurosci 29:9, 1532; Ramos-Nuñez 2017, Front Hum Neurosci 11, 420). Modularity measures the degree to which functional activity within a module of brain regions is more highly correlated than activity between modules, and flexibility measures the likelihood that brain regions change their module allegiance. Here, we investigated whole-brain network modularity and flexibility while subjects actively listened to a variety of auditory pieces that varied in cultural familiarity and emotivity. We found that low modularity subjects had fairly dynamic networks that adapted to process the culturally familiar and unfamiliar pieces. High modularity subjects had a more stable network organization and adapted modularity only during the unfamiliar pieces. Additionally, a strong negative correlation between modularity and flexibility was linked to processing culturally familiar audio with a clear meaning, versus processing music and speech that were unrecognizable. Our results suggest that the dynamical systems approach previously used (Ramos-Nuñez 2017) is not sufficient to explain the complex relationship between modularity and flexibility, and that new theory is need. This work also paves the way for creating individualized music therapy interventions.

O-4.5 – Quantifying Gas Phase Molecular Constituents Using Frequency-modulated Rotational Spectroscopy

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Frequency-modulated rotational spectroscopy is a powerful technique for detection of gas phase species. However, over the past several decades, it has been primarily used for qualitative analysis rather than quantitative analysis due to the complicated peak broadening mechanism, asymmetric peak shape and unclear dependence of signal intensity on source power. Here, we have developed an instrumental set-up and introduced a quantitative analysis procedure based on the Voigt peak model for frequency-modulated rotational spectroscopy. Gas molecules with partial pressure ranging over 3 orders of magnitude can be quantified with less than 4.1% error as was underpinned by the abundance analysis of N_2O isotopologues, featuring the unprecedented ability of this technique to pinpoint the position of ^{15}N isotope in N_2O molecule. Quantification of one molecule with another was also proved feasible with the cross-calibration technique, making it possible to circumvent the memory effect of adsorptive molecules. The detection limit of this technique was determined to be on the order of hundreds of femtomolar, demonstrating that this technique could be an important addition to the instrumentation options available for quantitative gas-phase detection.

Graduate Student and Postdoctoral Researcher Poster Sessions

GP-A Poster Session

GPA-01 – Millimeter-wave transitions in Sr Rydberg atoms

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Transitions between Rydberg states can be driven very efficiently with millimeter-wave radiation. This has been used for coherent control of electronic Rydberg states and for precision measurements. In this poster we will describe progress towards driving millimeter-wave transitions in ultracold Sr Rydberg atoms. We focus on millimeter-wave excitation of 5*sns* $^3S_1$ Rydberg states to nearby ^3Pj states and $^3S_1/^3Dj$ states with one and two-photon excitation respectively. A major motivation of the development of this technique is the study of vibrational wave-packet dynamics in ultralong-range Rydberg molecules.

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GPA-02 – Highly Dispersed Carbon Nanotube Epoxy by 3D Printing

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Carbon nanotubes (CNTs) are an extensively studied material which demonstrates robust mechanical and electrical properties. Although CNT composites are strong candidates for industrial application in aerospace, MEMs, robotics, and communication technology, CNT composites are difficult to process without specialized equipment. Mold casted CNTs demonstrate poor dispersion over 0.4wt% CNT due to van der Waals forces which cause CNT agglomeration. Furthermore, mold casted CNT composites are subject to void formation during fabrication, high viscosity composites are difficult to produce complex geometries, and CNT wetting is difficult to attain. Uniform CNT dispersion, high CNT wetting, and CNT alignment in composite materials have been previously been demonstrated by chemical treatment or functionalization of CNTs at the cost of mechanical or electrical properties of pure CNT. However, Advancements in additive manufacturing enables researchers to affordably investigate nearly any composite material. CNT epoxy composites have sparked interest in aerospace and other technologies as light weight structural, conductive, or EMI shielding materials, however, processing makes them impractical solutions over carbon fiber composites. Printing CNT epoxy composites shows promise to overcome many obstacles which prevent CNT epoxy composites from surpassing carbon fiber epoxy composites. Here we present a void reduced, uniformly dispersed, highly wetted CNT epoxy composite which eliminates the need for molds and chemical treatment.

GPA-03 – Development of a neutral peptide-based scaffold for mesenchymal stem cell preservation

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Mesenchymal stem cells (MSCs) have promising characteristics for cell therapy applications. However, there is a growing need to improve the methods for stem cell preservation, to minimize the loss of cell viability and differentiation potential during transportation and long-term cell storage. Induction of quiescence offers an alternative for common cryopreservation, and biomaterials such as multi-domain peptides (MDPs) can be useful for this application. $O_5(SL)_6O_5$, a hydroxyproline-based MDP developed by Tania Lopez-Silva, has been reported to preserve cell viability without promoting proliferation. The present study aims to further investigate the ability of $O_5(SL)_6O_5$ to preserve different cell types by inducing quiescence, as well as test the biocompatibility of the peptide as a scaffold for encapsulation of MSCs. Murine fibroblasts (NIH-3T3 cells) or MSCs were encapsulated in MDP hydrogels using 1% of the peptide in a 50:50 sucrose/HBSS solution. Live/dead staining and actin staining were performed to determine cell viability and morphology of the cytoskeleton, considering timepoints between day three and day fourteen for $O_5(SL)_6O_5$ and other MDPs. Positively charged MDPs, as well as those with RGDS mimic attached, promoted cell adhesion and proliferation, whereas negatively charged MDPs and $O_5(SL)_6O_5$ promoted a rounded morphology with low proliferation.

GPA-04 – Faster Compressive Hyperspectral Video Microscopy

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Compressive imaging is a technology based on the inherent redundancy in most natural scenes. Though compressive imaging is faster in acquisition, the iterative L1 signal reconstruction required adds a computational burden. For example, in compressive hyperspectral video for sum-frequency generation (SFG) microscopy, the computational cost becomes higher due to the increased dimensionality of the reconstructed spectral bands in the datacube. The Sum-To-One (STOne) transform is a sensing matrix previously designed specifically for compressive video which we now apply to compressive SFG. In addition, by using the multi-resolution properties of the STOne transform, we can reconstruct a foveated image significantly faster relative to the full resolution image reconstruction. By exploiting parallel computing, this method can also be extended to full resolution image reconstruction as a collection of foveated regions stitched together. When we used this method on hyperspectral video measurements, the experimental data showed a reduction in reconstruction time while essentially preserving reconstruction quality.

GPA-05 – Observation of trochoidal dichroism

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Matter's sensitivity to light polarization is classically characterized by linear and circular dichroism. Nanophotonics now provides the tools to strongly confine and focus light on the nanoscale, such as the evanescent near-fields surrounding waveguides in photonic circuits. However, matter's inherent sensitivity to the full range of polarization states that can be found in evanescent waves has not been explored, leaving an opening for observing novel light-matter interactions. Trochoidal, or cartwheeling, field motion is relatively unexplored and can be found in intereference fields, tightly focused gaussian beams, and evanescent waves produced via total internal reflection. Unlike the helical field motion of circular polarization, trochoidal polarization consists of rotational motion confined to a plane. We develop the trochoidal analog of the Born-Kuhn model for understanding circular dichroism, where a key distinction is the planar confinement. This system is experimentally realized via a coupled pair of plasmonic dipole scatterers. We find that the plasmon mode hybridization between the pair depends on the rotational direction of the trochoidal excitation field. This observation constitutes a novel geometric basis for dichroism that fundamentally differs from circular dichroism, which we name trochoidal dichroism. Future applications of trochoidal dichroism could involve radiative reporting of near-field polarization phenomena and interfacial molecular geometry, accessing previously unseen information due to this unique polarization.

GPA-06 – Thermal Focusing at the Nanoscale

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Water treatment technologies have increasingly been incorporating nanotechnology to increase efficiency and reduce wasted resources. Plasmonic nanomaterials are particularly attractive for this purpose, due to their strong light-matter interactions that can create localized photothermal heating. The local temperature increase can vaporize water without the need to boil the bulk solution. This project aims to utilize light interaction with an array of nanostructures to generate large localized temperatures, which can be used for both high temperature chemical reactions and solar steam generation (as an alternative desalination method). This work utilizes antenna-reactor nanostructures for photothermal heating. The antenna nanostructure captures incident light and focuses it on the nearby reactor, causing it to heat up. The system presented in this work uses gold bowtie antennas with a gold nanorod reactor. The bowtie antenna, which looks like two triangles facing each other with a nanoscale gap in between, scatters the radiation and generates a large electric field in the nano-gap. This effectively amplifies the intensity of the incident laser by over an order of magnitude. The nanorod is placed in this gap, sitting in the hotspot of the near-field enhancement generated by the antenna, and heating hundreds of degrees, according to theoretical simulations. The antennas are connected to the underlying conducting substrate to remove their heat, whereas the nanorod is thermally insulated to maintain the generated high temperatures. The structures were fabricated using electron-beam lithography and experimental results show the gold nanorod melting to a nanosphere, while the bowtie antennas retain their shape.

GPA-07 – Cisplatin Encapsulated within Gadonanotubes as a New Advanced Theranostic Agent Against Cancer

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Due to their interesting inherent magnetic, optical, and electrical properties, there are many reasons for employing carbon nanotubes (CNTs) for theranostic applications in medicine. Herein, we report the preparation, characterization, and *in vitro* testing of a new CNT-based theranostic agent having cisplatin (cis-diamminedichloroplatinum(II), CDDP) encapsulated within the advanced MRI contrast agent known as Gadonanotubes (GNTs) for the treatment of two different breast cancer cell lines (MCF-7 and MDA-MB-231). The new agent, abbreviated as CDDP@GNTs, has been shown to have increased therapeutic efficacy comparing to CDDP@CNTs. Complete characterization of the CDDP@GNTs has been accomplished using high-resolution transmission electron microscopy (HRTEM), scanning electron microscopy equipped with energy dispersive spectroscopy (EDS), inductively-coupled optical emission spectrometry (ICP-OES). Furthermore, the anticancer activity of the CDDP@GNTs has been evaluated against MCF-7 and MDA-MB-231 and showed to have significantly enhanced cytotoxicity over free CDDP after 48 h. The T1-weighted MRI of CDDP@GNTs (115 $mM^{-1}\ s^{-1}$ per Gd^{3+} ion at 1.5 T/RT) did not show any loss of MRI efficacy compared to reported values for the GNTs alone (90-160 $mM^{-1}\ s^{-1}$). In summary, CDDP@GNTs has considerable potential as new advanced theranostic agent against cancer.

GPA-08 – Magnetic anisotropy in RRh3Si7 single crystals (R = Gd-Yb)

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The highly localized f-electrons in the lanthanide metals give rise to very interesting properties such as Kondo effect and RKKY effect. Among numerous rare earth compounds, RRh3Si7 (Gd-Yb) attracts extensive attention due to its unique magnetic properties. Like other rare earth compounds, the ionic radius of the rare earth element decreased with increasing atomic mass due to lanthanide contraction. However, the magnetic ordering temperature has no trend and no theory can explain the phenomenon yet. The objective of this work is to analyze the magnetic and the electronic properties through magnetization, heat capacity as well as the electric resistivity measurements of RRh3Si7 (R = Gd-Lu) compounds. We find competition between different energy scales including magnetic interactions, crystal electric field effect or Kondo energy.

GPA-09 – Exploring relative charge and energy transfer efficiencies to tune and predict chemical reactivity of hybrid plasmonic/organic semiconductor nanomaterials

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Recently, our research group has developed an electrochemical deposition method to fabricate hybrid plasmonic/organic semiconductor nanoelectrodes. Single particle spectroscopy was used to characterize the energy transfer efficiencies of the hybrid structures by recording the surface plasmon resonance energy linewidth change during in situ polymerization. While this preliminary data provides information about the mechanism of energy transfer, it does not establish how metal-semiconductor combinations with differing donor-acceptor absorption overlap and electronic band alignments impact charge and energy transfer efficiencies. A strategy to predict and tune internal energy conversion ratios in hybrid plasmonic-semiconducting nanostructures to subsequently drive photochemical and electrochemical reactions has yet to be proposed. In this work, we complement results from single particle measurements with ensemble measurements to determine the factors governing each mechanism. Specifically, we quantify how different ratios of energy and charge transfer impact photoreaction dynamics in a series of different gold nanoparticle/conductive organometallic polymer heterostructures.

GPA-10 – Generating Vacuum Ultraviolet Light at 185 nm via Third Harmonic Generation in a Titanium Dioxide Metasurface

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All-dielectric metasurfaces have recently been shown to provide an excellent platform for harmonic generation due to their low-loss nature and ability to strongly confine visible or near IR light within their nanoresonators. In this work, we present a metasurface consisting of titanium dioxide (TiO_2) nanostructures for third harmonic generation. It was designed to enhance the generation of light at the third harmonic frequency of an ultrafast laser by providing electric field

enhancement at the fundamental laser wavelength. To do this, the geometric design parameters were tailored to achieve a photonic resonance around the pump wavelength of 555 nm. In this way, VUV light at a wavelength of 185 nm was generated. In particular, the metasurface showed an enhancement factor of around 180 compared to an unpatterend TiO_2 thin film of the same thickness. This enhancement is evidence of strong electric field enhancement within the nanostructures. A detailed mode analysis revealed that the origin of this is due the presence of an anapole resonance in the vicinity of the pump wavelength.

GPA-11 – A quantum algorithm to count weighted ground states of classical spin Hamiltonians

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Counting ground states—minimum energy configurations of a Hamiltonian—plays an important role in science and engineering, from estimating residual entropy in physical systems, to counting solutions of constraint satisfaction problems relevant to engineering applications. While quantum algorithms such as adiabatic quantum optimization (AQO) and quantum approximate optimization (QAOA) can minimize Hamiltonians, they are inefficient in counting the minimum energy configurations.

We modify AQO and QAOA to efficiently count the ground states of classical Hamiltonians. Additionally, we extend our solution to cases where the ground states are counted with different weights attached to them. As a concrete example, we show how our algorithms can be used to count the weighted fraction of edge covers on networks—which has important applications in determining the reliability of natural and engineered complex systems—with user-specified confidence on the relative error of the weighted fraction. We analyze the complexity of our algorithms, via analytical predictions for AQO and numerical calculations for QAOA on a broad class of edge cover problems, and compare to optimal Monte Carlo simulation (OMCS), which is among the best available classical algorithms. We also test our algorithms on counting solutions of other problems of interest, such as maxcut, maximal independent set, and exact covers.

We show that for large problem instances with small weights on the ground states, AQO does not enjoy a quantum speedup over OMCS, but QAOA can potentially achieve a sub-quadratic speedup, when the weighted count of minimum energy configurations is small. Our work opens avenues to employ current noisy intermediate-scale quantum hardware for solving ground state counting problems on small instances, and can lead to identifying more problem classes with quantum speedups.

GPA-12 – When will the cancer start? Elucidating the correlations between cancer initiation times and lifetime cancer risks

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Cancer is a genetic disease that results from accumulation of unfavorable mutations. As soon as genetic and epigenetic modifications associated with these mutations become strong enough, the uncontrolled tumor cell growth is initiated, eventually spreading through healthy tissues. Clarifying the dynamics of cancer initiation is thus critically important for understanding the molecular mechanisms of tumorigenesis. We developed a new theoretical method to evaluate the dynamic processes associated with the cancer initiation. It is based on a discrete-state stochastic description of the formation of tumors as a fixation of unfavorable mutations in tissues. Using a first-passage analysis the probabilities for the cancer to appear and the times before it happens, which are viewed as fixation probabilities and fixation times, respectively, are explicitly calculated. Our model predicts that the slowest cancer initiation dynamics is observed for neutral mutations, while it is fast for both advantageous and, surprisingly, disadvantageous mutations. The method is applied for estimating the cancer initiation times from experimentally available lifetime cancer risks for different types of cancer. It is found that the higher probability of the cancer to occur does not necessary lead to the fast times of starting the cancer. Our theoretical analysis helps to clarify microscopic aspects of cancer initiation processes.

GPA-13 – Hot-carrier-Mediated Photocatalysis by Al@TiO2 Core-Shell Nanoparticles

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Plasmon-induced hot carriers with excess kinetic energy have been demonstrated to facilitate photocatalytic processes. To effectively generate and utilize hot carriers, antenna-reactor heterostructures are developed by combining plasmon nanostructures and catalytic materials with active surface sites for chemical reactions. The interface between plasmonic and catalytic materials, as well as their individual morphology, is crucial for efficient charge transfer. Here we introduce Al@TiO2 core-shell nanoparticles as a hot-carrier-mediated antenna-reactor for the photoreduction of 4-aminophenol. During Al@TiO2 synthesis, the native oxide layer of Al nanocrystals which impedes the charge transfer pathway is removed and replaced by a semiconducting TiO2 shell. The Al-doped TiO2 interlayer formed at the interface assures close contact and allows almost barrierless charge transfer between Al and TiO2. In such a geometry, the plasmonic Al core generates energetic hot carriers under ultraviolet to visible illumination through both nonradiative plasmon decay and direct excitation of interband transitions. The hot carriers subsequently transfer to the TiO2 shell to promote chemical reactions. The Al@TiO2 heterostructure, as an antenna-reactor, demonstrates high photocatalytic efficiency and provides a low-cost solution for the future design of plasmon-induced photocatalysts for visible-light-driven reactions.

GPA-14 – Understanding Collagen Interactions to Predict the Stability of Collagen-Mimetic Peptides

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Collagen has been studied using collagen-mimetic peptides (CMPs) for over twenty years. CMPs mimic the structure of collagen and are effective for modeling binding domains and collagen-related diseases. Most of these models have utilized homotrimeric triple helices, however, due to the nature of many natural collagens, a representative picture of these systems demands the use of heterotrimers. Heterotrimers introduce a problem of competition between various triple helical species, each with comparable thermal stability. Thus, new strategies for assessing and designing CMPs are important for understanding and controlling competitive arrangements. Researchers have made preliminary efforts to understand the effects of amino acid content on the structural stability of CMPs. Our efforts to expand on this include (1) a rigorous study of amino acid propensity and pair-wise interactions and (2) the design of an algorithm to predict CMP triple helix thermal stability. To that end, 50 peptides were synthesized to study 33 amino acid pairwise interactions. The interactions studied sample hydrophobic, charge-pair, and cation-π interactions. The deconvoluted substitutions' and interactions' stability effects were combined with information from literature to design our algorithm. 391 triple helices with published melting temperatures were harvested from the literature to test the accuracy of the algorithm. The predicted values matched the published melting temperatures with an R^2 of 0.94.

GPA-15 – Fibronectin's surface-induced unfolding is restricted by the simultaneous but not sequential introduction of competing serum albumin

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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. Many traditional experimental approaches cannot simultaneously measure the behavior of a single protein in a physiologically complex environment, meaning that effects due to competing protein crowding are often not considered. In the current work, we directly measure the unfolding of dye-conjugated fibronectin (Fn) in varying conditions of crowding with human serum albumin (HSA) using single molecule high resolution imaging with photobleaching, a technique that is well suited for monitoring the behavior of single proteins in a complex environment. We find that Fn attains a more compact structure in the presence of crowding HSA. We also report that HSA does not significantly influence Fn conformation if it is sequentially introduced rather than simultaneously. Our findings confirm that Fn conformation is dependent on macromolecular crowding and support earlier work that has suggested that protein crowding induces changes in Fn's physiological activity.

GPA-16 – Expansion of an Ultracold Plasma with an Exponential Density Profile

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Ultracold neutral plasmas (UNPs) provide a powerful platform for studying a wide range of fundamental plasma processes, including the expansion of a plasma into surrounding vacuum. Most previous experiments with UNPs have been performed with plasmas possessing a Gaussian density profile, for which the expansion is well characterized and provides a useful diagnostic of initial electron temperature and three-body recombination in the plasma. A defining characteristic of a Gaussian plasma is self-similar expansion, which gives important time scales and length scales. While Gaussian plasmas are well understood, other interesting initial profiles have not been explored. This poster describes the expansion dynamics observed for UNPs formed by photoionizing a cold atomic gas from a quadrupole magnetic trap, which creates a plasma with an initial exponential, or "cuspy," density distribution. We find that while the cuspy plasma does not self-similarly expand and other expansion details are different, important expansion time scales and length scales can be identified that are similar to the situation for a Gaussian plasma.

GPA-17 – Highly sensitive photoacoustic multicomponent gas sensor for SF_6 decomposition online monitoring

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A ppb-level photoacoustic multicomponent gas sensor system for sulfur hexafluoride (SF_6) decomposition detection was developed by the use of two near-infrared (NIR) diode lasers and an ultraviolet (UV) solid-state laser. A telecommunication fiber amplifier module was used to boost up the excitation optical power from the two NIR lasers. A dual-channel high-Q photoacoustic cell (PAC) was designed for the simultaneous detection of CO, H_2S, and SO_2 in SF_6 buffer gas by means of a time division multiplexing (TDM) method. Feasibility and performance of the multicomponent sensor was evaluated, resulting in minimum detection limits of 435 ppbv, 89 ppbv and 115 ppbv for CO, H_2S and SO_2 detection at atmospheric pressure. The optimal design of the excitation optical sources and the detection module offers a sensitive, small-size and cost-effective SF_6 decomposition sensor, which is very practical for online monitoring of an electric power system.

GPA-18 – Spatiotemporal Single Particle Tracking Using Point Cloud Clustering

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Single particle tracking algorithms have two well-known issues: photoblinking and trajectory overlap. Traditional methods solve these issues using *a priori* knowledge of the particle's motion, introducing bias. Data driven approaches fill these knowledge gaps by relying on internal consistency determined by the data itself, thus avoiding bias. We present an application of a data driven method, point cloud clustering, to 3D single particle tracking. Our novel approach uses 3D particle localizations provided by the Alternating Direction Method of Multipliers to build a point cloud which we condense into particle trajectories. Point cloud segmentation predicts which points belong to each trajectory, thereby interpolating through photoblinking events and untangling trajectory overlaps. We illustrate the method's effectiveness on simulated trajectories of varying complexity. Future applications include tracking intracellular phenomena which exhibit high degrees of both photoblinking and trajectory overlap.

GP-B Poster Session

GPB-01 – Single Particle Studies on the Degradation of Gold/Silver Alloy Nanoparticles

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Plasmonic metal nanoparticles have attracted great attention for a broad range of sensing and catalyst applications. While gold nanoparticles provide excellent stability in a broad range of conditions, other metal nanoparticles suffer from instability towards oxidation. One common approach to prevent nanoparticle oxidation is by coating the particles in protective layers such as oxides. However, this surface layer will often change the surface chemistry and passivate the nanoparticle towards other reactions. Here, we present single particle studies of gold/silver alloy nanoparticles prepared by laser ablation from alloy foils. This ligand free preparation ensures a completely bare and unfunctionalized surface and a homogenous distribution of gold and silver in the alloy particle. Through hyperspectral imaging before and after a three day aging period we find a heterogeneous redshift and linewidth broadening for particles that contain 90% silver, indicating oxidation of the silver content, as confirmed by EDX measurements. SEM also showed morphological changes associated with oxidation. Correlated hyperspectral imaging and EDX revealed that plasmon broadening and red-shift can be directly correlated with silver leaching out of the particle. This work presents an easy in-situ method to study nanoparticle degradation through single particle spectroscopy. Future work will focus on dynamic studies of bare and aptamer functionalized silver nanoparticle oxidation in electrolyte solutions.

GPB-02 – Graphene Coated Vanadium Pentoxide: A prospective electrode material of high capacitance for intercalation based brackish water desalination

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This work introduces the use of graphene-coated vanadium pentoxide (V2O5) as electrodes for capacitive desalination of low molarity saline water. While utilizing the honeycomb structure of V2O5 grown on stainless steel (SS) mesh as the electrode, the electrical double layer formation along with ion intercalation is observed during desalination cycles leading to an improvement in the removal of NaCl from the solution. The capacitance tests through a 3-electrode setup of V2O5 grown on stainless steel mesh and coated with graphene shows high capacitance values, 500 F/g which is due to the presence of both electrical double-layer capacitance and pseudocapacitance. The CDI process shows cell performance of over 50 cycles at 5, 10- and 15mM concentration with a salt removal capacity of12.5 mg/g. This new method of utilizing the faradaic and non-faradaic process for desalination pave a way towards more efficient, cost-effective sea water purification systems.

GPB-03 – Quantitative description of nanorod aggregates in scanning electron microscopy images

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Aggregation is a major concern when working with colloidal suspensions of nanoparticles. Despite extensive research into the conditions in which nanoparticle aggregation occurs, little has been reported on the inter-particle structure of the aggregates that do form. We have developed two methods for quantitatively measuring the physical structure of nanoparticle aggregates: an algorithm for segmenting dense aggregates measured with scanning electron microscopy (SEM) and an order parameter for characterizing the side-by-side structure. The segmentation algorithm is an application of the marker-controlled watershed method where the nanoparticle markers are isolated through a series of image-processing steps. We have successfully segmented individual nanoparticles in aggregates under conditions with dim boundaries and intensity variation that preclude the use of other methods. Segmented SEM images can be used to quickly calculate the side-by-side order of a large number of aggregates. We report on the differences in gold nanorod side-by-side order after induced aggregation with bovine serum albumin and salt (NaCl) Future work will see these methods implemented with an open-source, user-friendly interface to provide quantitative image processing tools for researchers to characterize aggregate structure with high throughput.

GPB-04 – A ReaxFF Investigation of Adhesion Properties at Si/Polymer Interfaces

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High capacity lithium-ion battery anodes based on silicon undergo large volume fluctuations during operation that can compromise the structural integrity of the electrode. This issue can be mitigated by using flexible polymers to encapsulate the active Si material so that the electrode can accommodate significant volume expansions and contractions. Such designs require a stable interface between the polymer and Si that can undergo repeated deformations during battery cycling. To help design such interfaces, we have developed a ReaxFF force field to investigate the interfacial adhesion properties of the Si/polymer interfaces at the atomistic scale. We consider three C/N/H based polymers in this study that

have been shown to improve the battery performance: polyacrylonitrile (PAN), pyrolyzed polyacrylonitrile (PPAN) and polypyrrole (PPy). Molecular dynamics simulations with the newly developed ReaxFF parameters show that single chains of PPy bind more strongly to Si compared to those of PAN or PPAN, which is validated by adsorption energies computed with density functional theory (DFT). This trend reverses when considering the interface between the bulk polymer and Si, where PPy binds least strongly to the surface. We show that this reversal is caused by the interaction mechanism of individual polymer chains at the interface, where the strong and parallel binding of the first layer of PPy chains prevent the next layer of chains from accessing the surface. The methods and simulation tools presented here prove to be significant resources for gaining insight into atomic-scale understanding of the interfacial phenomena of other Si/polymer composite materials.

GPB-05 – Towards predictive chromatography: Computationally directed separations for efficient drug design and production

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Chromatographic purification of protein based drugs is a complicated enterprise lacking rigorous theory to predict the outcome of a separation. Many theories have been posited to describe the separatory action of chromatography. All require empirically derived assumptions that prevent accurate prediction of the final elution profile. This gap in predictive power reduces chromatographic column optimization to costly, iterative empirical testing, making the process of designing new drugs inefficient. Specifically, current theories fail to consider rare events in the column that lower separation efficiency. Uniting single molecule experimental data with the complementary Giddings and Eyring model of chromatography can rectify this gap of knowledge. To achieve this union, we construct an extensible Monte Carlo simulation framework that can anticipate mechanisms that lower separation efficiency on a protein-by-protein basis. Reconstructing the ensemble chromatographic lineshape from single protein adsorption histories (shown below) identifies undesirable chemical effects and enables pre-emptive adjustments of column chemistry before implementation at the industrial scale. Anticipating problematic chemical phenomena via single molecule powered predictive theory points to drug-specific engineered chromatographic columns optimized via machine learning. Doing so marries nanoscale empirical insights with the powers of modern computation to simulate macroscale reality.

GPB-06 – Sinter-Cracking: Initiation, Propagation, and the Stress Field

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Sintering is a heat treatment used to consolidate a powder material into a continuous solid body. The large shrinkages involved can lead to internal stresses in the sintering material, which in turn can lead to cracking when amplified by stress concentrating features. This is particularly problematic for a powder material aggregate possessing a complex design geometry, such as can be produced by binder jet 3D printing. We investigate sinter-crack initiation and growth using the discrete element method to simulate the evolution of sintering specimens having traditional fracture mechanics geometries and known stress parameters. The method allows a direct look at the stress state in the sintering material, revealing how stress concentrates ahead of a sinter-crack, and that the stress field can be related to that of creep-cracking in fully dense materials. We investigate sinter-cracking experimentally using binder jet 3D printing and *in situ* imaging; we find that crack initiation is mitigated or prevented for flaws below a critical size or stress concentration factor. The ability to predict sinter-crack behavior can lead to design guidelines for avoiding the problem of cracking during sintering.

GPB-07 – Scalable Plasmonic Metasurfaces

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Plasmonic metasurfaces have been demonstrated for a wide range of functionalities in a variety of fields. From second- and third- harmonic generation to enhanced spectroscopies to photodetectors, plasmonic structures and metasurfaces have provoked profound research interest. Central to these research breakthroughs seeing widespread adoption is the ability to produce such structures at scale. In this work, we present a potential route forward to achieving large-scale manufacturing of plasmonic metasurfaces. Using a combination of colloidal nanoparticle synthesis, electrophoretic deposition, and nanoimprinting we demonstrate the ability to create nanopatterned surfaces over several square inches, with the potential to be scaled further to square feet. We believe that this work presents a path forward towards real-world applications for a variety of plasmonic-enhanced metasurfaces.

GPB-08 – Enhanced reversibility in anode-free Li metal batteries using laser induced silicon oxide layer

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Rechargeable Li metal anode is a key technology for future high energy density batteries. Practical issues hindering Li anodes are the formation of Li dendrites and the production of inactive Li pieces during plating and stripping process, which can cause short circuit, thermal runaway and low coulombic efficiency (CE). Here, we study the use of a laser-induced silicon oxide (SiO_x) layer derived from a commercial tape (Kapton) to prevent the formation of Li dendrites and improve reversibility of anode-free Li metal batteries. In this process, the silicone-based adhesive of the tape is converted by an IR laser to a homogeneous silicon oxide (SiO_x) layer deposited directly over the current collector. The laser-induced SiO_x coating results in superior performance by suppressing the formation of Li dendrites and presenting higher coulombic efficiency (CE) and cycling stability compared to the electrode without coating. The aspect ratio of deposited Li can be detected, which uncovers the different mechanism of Li deposition after introducing SiO_x layer. Compared with other methods of coating, the use of laser to produce electrode coatings is dry, fast and avoids the use of organic solvents and time for drying. The improved performance with SiO_x coating represents a progression in the search for reliable Li metal cells.

GPB-09 – Ab initio investigation of Nitrite Reduction to Ammonia at Room Temperature through Aqueous-phase Rhodium Catalysis

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Nitrogen pollution is an increasing environmental concern as we continue to discharge reactive N-containing species into the environment, mostly as nitrate or nitrite (NO_3^-/NO_2^-). This is an unintended consequence of industrial nitrogen fixation processes like Haber-Bosch. Transition metal catalysts, such as Pd, are known to be effective for removing NO_3^-/NO_2^- from water by reducing it to harmless N_2. The mechanism of nitrite reduction is well established on metals like Pt and Pd at low

pH, but the chemistry of nitrite reduction at higher pH conditions is not well explored. In this work, we elucidate NO_2^- reduction mechanisms on Pd and Rh catalyst at varying pH conditions. Experimentally we found that Pd reduces NO_2^- to N_2 with very high selectivity at low pH conditions but becomes inactive with an increase in pH. Conversely, Rh is inactive at low pH and is active at high pH (and forms NH_3 instead of N_2). To explain the observed differences in NO_2^- reduction, we employed density functional theory (DFT) to elucidate reaction mechanisms by calculating reaction free energy changes and associated activation barriers. We found that HNO_2 readily dissociates on Pd and Rh catalysts, covering the surface with stable NO* species. Microkinetic models demonstrate that this NO* species poisons the Rh catalyst surface at low pH, which is a result of rapid HNO_2 dissociation. As pH increases, the activation barrier for HNO_2 dissociation increases, thus relieving the surface poisoning effect. These computational predictions were confirmed by *in aqua* surface-enhanced Raman spectroscopy (SERS) measurements, which demonstrate that NO* is present on the Rh surface only at low pH.

GPB-10 – Active control of protein dynamics on pH-responsive polymer hydrogels

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Protein confinement at the porous chromatographic support leads to anomalous confined diffusion affecting the efficiency of molecular separations. Molecular-level understanding and control over such complex dynamics are needed for predictive applications. Cross-linked hydrogels made of stimuli-responsive polymers provide unique control over their physio-chemical properties by spatial and chemical transformation with environmental changes. These stimuli-driven transformations generate a dynamic heterogeneity of hydrogels' physio-chemical properties and are the driving forces behind their underlying surface chemistry. Fluorescence correlation spectroscopy combined with Super-resolution Optical Fluctuation Imaging (fcsSOFI) is ideal to understand the complex dynamic behavior of proteins and characterize porous polymer surface. Herein, we use fcsSOFI and single particle tracking to understand the dynamics of a model protein lysozyme on the pH-responsive hydrogel surface and inside the hydrogel pores. Single protein tracking analysis reveals the dynamic reversibility of the hydrogel polymer in response to the pH change of the environment. Chemical heterogeneity of the surface and geometrical confinement dictates the dynamic hoping behavior of proteins at the complex nanogel surfaces. The single-molecule picture of these complex processes and active control of protein dynamics 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.

GPB-11 – Polymer Pen Lithography as a New Strategy for Nanoparticle Fabrication

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Nanoparticles offer many potential applications due to their unique properties, but this is hindered by the need for precise control of their size and morphology. Nanofabrication strategies, such as electron beam lithography or dip-pen nanolithography, have shown ability to comply with these requirements. However, these strategies often come with high expenses while also failing to provide a high throughput. Other strategies, like micro-contact printing or photolithography, can deliver high throughput, but lack the necessary flexibility and precision.

A new alternative to these techniques is Polymer Pen lithography (PPL). PPL is a molecular printing method, in which molecules are directly transferred from elastomeric, pyramidal-shaped tips onto to a substrate with sub-100nm resolution. The tips are sharp, robust and can be used with a variety of inks, ranging from small molecules to polymers and biomolecules. PPL uses arrays of up to 2.80 million tips, which ensures high throughput in a single printing process. The usage of piezo stages enables high control of the tip positions and allows for precise material deposition. PPL can be conducted with a single instrument that is easy to operate and does not need further equipment or materials. Therefore, PPL has the potential to provide a fast and affordable way for the fabrication of complex nanoparticles in the future. We will show our recent results on fabricating gold nano discs using PPL.

GPB-12 – Covalent Capture of the Collagen Triple Helix

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Collagen mimetic peptides (CMPs) are used to study the structure and function of natural collagens. However, issues involving folding equilibria—slow folding and low trimer concentrations—are particularly problematic for applications involving low peptide concentrations. Previous studies have shown that pairwise interactions between lysine and aspartate or glutamate can be used in CMPs to stabilize the desired composition and register of the triple helix. After selective formation of the desired heterotrimer, the assembly can be covalently captured using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) and 1-hydroxybenzotriazole (HoBt) to form amide bonds between the amine and carboxylate side chains. Herein we have utilized an AAB heterotrimer to demonstrate both lysine-aspartate and lysine-glutamate bond formation. The resulting covalently captured system is shown to address the CMP issues involving folding equilibria. Size-exclusion chromatography shows the triple helix can be isolated, removing all monomer from the system. Circular dichroism thermal refolding experiments show nearly immediate recovery of triple helical structure after covalent capture. Comparing side chain length, glutamate shows amide bond formation more rapidly compared to aspartate and does not lead to distort the secondary structure. This covalent capture of the collagen triple helix will be useful in applications involving CMPs. For instance, a covalent capture region could be attached to a region of interest on a CMP. After covalent bond formation, the CMP trimer could be purified and used in applications such as activation or inhibition of collagen-binding receptors or for use in biomaterial development.

GPB-13 – ALD-modified $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (NMC) paired with Macro-Porous Silicon for Li-ion Batteries: An investigation on Li trapping, Resistance rise and cycle-life performance

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Li-ion battery (LIB) electrode materials like Silicon anode and NMC cathode have gained tremendous research interest due to the high energy density, which is one of the significant properties essential for energy applications. However, the unstable electrochemical performance Si anode & NMC cathode has created hindrance to the practical utility of these materials in LIB applications. Our earlier research reported the half-cell performance of micron-sized porous Si/polyvinyl pyrrolidone (pSi) composite anode design with improved cycle life and stability using a capacity-controlled charging strategy. The hydrogen fluoride mediated capacity fading of NMC cathodes in $LIPF_6$ based electrolyte is a well-known phenomenon that is attributed to the gradual disintegration NMC structure leading to retarded electrochemical performance. Herein, we report a full-cell design using a pSi anode and alumina coated NMC cathode that provide cycle stability by means of capacity-limited charging. The proposed Si–NMC full-cell design with alumina passivation on cathode has exhibited a stable capacity of 1000 mAh/g, with 1.2 times higher energy density than the Si-NMC full-cell without cathode passivation. The role of alumina coating on the altered half-cell electrode charging mechanisms and the electrochemical full-cell reactions with Si anode were investigated systematically using various structural and chemical analysis. The alumina passivated Si-NMC full-cell designed in this study elucidated an interesting electrochemical behavior of Li-trapping and rapid rise in cell voltage, which shed light to the factors that need to be considered in the efficient utilization of Si-NMC battery for high energy applications.

GPB-14 – Photoassociation of Fermionic 87Sr Near the 5s5p(1P1) Asymptote

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The fermionic isotope of strontium, 87Sr, is of interest for the development of optical frequency standards and the study of quantum many-body phenomena. In many of these experiments, 87Sr is confined in an optical lattice. Detecting the presence of doubly occupied lattice sites is a valuable tool for studies of atomic gases in optical lattices, and this is typically done with photoassociation, in which two gound-state atoms in a scattering state are photo-excited to a molecular state. No resonance frequencies have been reported for transitions to molecular states of any excited electronic potential for 87Sr. Here we present results for photoassociation of 87Sr atoms via the 1S0 - 1P1 transition at 461nm ($\Gamma=(2\pi*30.5)s-1$), and plans to measure optical lengths for select photoassociation spectra.

GPB-15 – Quantitative comparison of adaptive sampling algorithms for protein dynamics and scalable execution with ExTASY

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Computer simulations of many biological processes are still out of reach despite parallelization, High-Performance Computers (HPC) systems and speed improvements with GPUs. In many cases "brute force" MD simulations are performed, but a more efficient sampling of the biological processes could increase the reachable biological timescales. Adaptive sampling methods prioritize the sampling of different parts of the protein process according to different algorithms. Here the quantitative comparison of different adaptive sampling algorithms is shown as well their scaling and the upper limit for the speed up with adaptive sampling. The user-friendly execution of adaptive sampling with the ExTASY framework is demonstrated on three proteins with the accurate recovery of the protein dynamics.

GPB-16 – Produced Water Treatment: Selective Electrosorption of Scale-forming Ions

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Water produced from oil and gas exploration activities is rich in divalent cations (Ca^{2+}, Ba^{2+}, Sr^{2+}) and anions (SO_4^{2-}). Reuse of this water causes scale formation throughout the exploration network, which affects the operation and requires maintenance and sometimes leads to temporary or permanent operation shutdown. Current technologies used for removal of these ions require a huge amount of chemicals, produce sludge or sometimes not very effective. In my work, I am developing an electrochemical ion separation technology to effectively and selectively remove those ions by using electrical energy, activated carbon powder and charged polymers. Activated carbon powder is first cast into thin sheets followed by surface modification with the sulfonated polymer layers. Such sheets are placed opposite to each other leaving a gap in between for contaminated water to flow. A DC voltage is applied across the pair of modified carbon sheets and target ions are selectively transported through the polymer layers and into the pores of the activated carbon, producing divalent ion deficient stream. Once the sheets are saturated with the ions, the applied voltage is removed and a

waste stream concentrated in divalent ions is produced. Hence this system is operated to selectively remove target ions by just using electrical energy in a cost effective and environmentally friendly manner.

GPB-17 – Detection of Oligomeric Amyloid Aggregates in Real-Time Using Metal Complexes

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The formation of oligomeric soluble aggregates is related to the toxicity of amyloid peptides and proteins which play an important role in Alzheimer's disease. Here we report the use of a pyrazinephenanthroline metal complex ($[Ru(bpy)_2(dpqp)]^{2+}$) to track the formation of amyloid oligomers in real-time using photoluminescence anisotropy. Our assays show that amyloid-β (Aβ) forms oligomers immediately after the assay is started reaching a steady state at ca. 48h. Other methods such as SDS-PAGE, DLS and TEM were used to monitor and confirm the formation of oligomers. The probe also showed to be effective to monitoring the formation of α-synuclein oligomers in real-time.

GPB – Encapsulated mesenchymal stem cells delivered to the heart reduce the effects of acute myocardial infarction in a rat model

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Every year 790,000 Americans suffer from Myocardial infarction (MI)[1]. Despite high incidence, available treatment methods often leave residual myocardial scarring which can frequently lead to ischemic heart failure – the third most common cause of death[2]. Herein we present a therapy that targets regeneration of cardiac muscle post-MI by delivering paracrine factors such as VEGF, HGF, and IGF-1 released by mesenchymal stem cells (MSCs). These factors have been shown to enhance cardiac function due to their ability to promote angiogenesis and reduce apoptosis in vivo. Current studies that use MSCs for restoration of cardiac function show great regenerative potential but have a limited duration of therapy due to the host immune response eliminating administered cells. In this study, we used an immunomodulatory alginate polymer to encapsulate MSCs that have been transduced to express Firefly luciferase, a bioluminescent reporter. We then surgically implanted the capsules in the pericardial sac of healthy Sprague Dawley rats and used small animal IVIS imaging to show localization of our therapy to the heart and sustained viability of cells over time. The results show that even after two weeks, the encapsulated cells remain viable and continue to respond to luciferin delivered through intraperitoneal injection. The success of our delivery platform eliminates the need for re-dosing and greatly enhances the ability of the paracrine factors to act locally on the damaged myocardial tissue long term. Future work will include the application of our therapeutic in an infarct model in order to show reduction in scar tissue via histology.

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