

# 7th Annual SCI Summer Research Colloquium

# | Oral Session A

Topological and Anomalous Hall effects driven by correlations in a square-net centrosymmetric Eu-based compound

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Since the discovery of the Hall effect in 1879 by Edwin Hall, scientists and engineers have used the simple principle of measuring the transverse voltage when a magnetic field is applied perpendicular to a current to characterize the mobility and carrier concentration. It did not take long for scientists to realize that there are other possible Hall contributions that can shed light on much more than mobilities and carrier concentrations. In modern condensed matter physics, the anomalous and topological Hall effects are attributed to non-zero Berry phase accumulated when a charged carrier traverses a closed path in a material. In the former, the Berry phase arises as the integral of the Berry curvature which can be regarded as a fictitious magnetic field in reciprocal space and depends solely on the band structure of the material. In the latter, the Berry phase accumulation happens in real space and is generated by non-coplanar spin textures.

In this talk I will present the results of my Hall measurements on the square-net centrosymmetric Eu based compound  $\text{EuGa}_2\text{Al}_2$ . There are only 3 known such compounds, all Gd-based, and the stabilization mechanism is hotly debated. I find a topological Hall effect pointing to the existence of non-coplanar spin textures, or even particle-like spin textures called skyrmions, which can be useful in the application of spintronic devices. This result may shed light on the stabilization mechanism for skyrmion systems in the centrosymmetric compounds (with a center of symmetry in the crystal structure). Furthermore, I discovered a large temperature dependent anomalous Hall conductivity, suggesting a large Berry phase accumulation, which could be explained either by the appearance of field induced Weyl nodes, or a charge-density wave. While the former has been suggested in other materials, the latter is a new mechanism which could be used as a principle for material design.

## 2D charge-density-wave material for tunable nanophotonics - 1T-TaS<sub>2</sub>

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### ABSTRACT

Light is a powerful tool in sculpting the energy landscape of strong correlations such as charge density wave (CDW) materials. Here, we study the incoherent light tunable optical properties of a 2D CDW material, 1T-TaS<sub>2</sub> in its commensurate (C-) CDW at low temperature and nearly-commensurate (NC-) CDW at room temperature. We hypothesize that the observed large tunability is a consequence of the rearrangement of CDW domains staking across layers. The temperature-dependent dynamics of tunability suggest that the mechanism of switching among stacking types could be explained by the classical nucleation theory. Our model based on the hypothesis agrees reasonably well with the experimental results, indicating the interdomain CDW interaction is a vital potentially knob to control the light-matter interaction in strongly correlated materials.

## Universal Thermodynamics of an $SU(N)$ Fermi-Hubbard model

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The  $SU(2)$  symmetric Fermi Hubbard model (FHM) plays an essential role in the understanding of strongly correlated fermionic many-body systems. When the system is in the one particle per site and strongly interacting limit  $U \gg t$ , it is effectively described by the Heisenberg Hamiltonian. In this limit, extending the typical  $SU(2)$  symmetry to  $SU(N)$  is predicted to give exotic phases of matter in the ground state, with complicated dependence of the ground state on  $N$ . The question we address in this talk is whether the situation is similarly complicated at temperatures at and above the superexchange energy. To answer this question we numerically explore the  $SU(N)$  FHM in a two-dimensional square lattice using determinant Quantum Monte Carlo and Numerical Linked Cluster Expansion. Our main finding is that for temperatures above the superexchange energy, where the different  $N$  systems are just dominated by short-range correlations, the energy, double occupancy, and kinetic energy collapse upon a simple rescaling with  $1/N$ . Although the physics in the regime studied is well beyond that captured by low-ordered high-temperature series, we show that an analytic description of the scaling is possible in terms of only one- and two-site correlations.

# Realizing Su-Schrieffer-Heeger topological edge states in Rydberg-atom synthetic dimensions

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Synthetic dimensions based on coupled Rydberg levels in ultracold atoms can be a powerful tool for quantum simulation. We demonstrate this platform by implementing the Su-Schrieffer-Heeger (SSH) Hamiltonian on a Rydberg strontium atom. The Rydberg levels are interpreted as synthetic lattice sites and the tunneling is introduced through resonant millimeter-wave couplings. The millimeter-wave amplitudes control the tunneling amplitudes whereas frequency detunings of the millimeter waves from resonance control the on-site potential. We attain a configuration with symmetry-protected topological edge states by using an alternating weak and strong tunneling pattern, with weak tunneling to edge lattice sites. The band structure is probed through optical excitation to the Rydberg levels from the ground state, which reveals topological edge states at zero energy. We verify that edge-state energies are robust to perturbation of tunneling-rates, which preserves chiral symmetry, but can be shifted by the introduction of on-site potentials. The scope of Rydberg-atom synthetic dimensions in realizing higher dimensional systems, non-trivial spatial and band structure topologies, artificial gauge fields and many-body physics with long-range interactions in optical tweezers will also be discussed.

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# Magnetic Control of Soft Chiral Phonons in PbTe

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PbTe crystals have a soft transverse optical phonon mode in the terahertz frequency range, which is known to efficiently decay into heat-carrying acoustic phonons, resulting in anomalously low thermal conductivity. Here, we studied this phonon via polarization-dependent terahertz spectroscopy. We observed softening of this mode with decreasing temperature, indicative of incipient ferroelectricity, which we explain through a model including strong anharmonicity with a quartic displacement term. In magnetic fields up to 25 T, the phonon mode split into two modes with opposite handedness, exhibiting circular dichroism. Their frequencies displayed Zeeman splitting together with an overall diamagnetic shift with increasing magnetic field. Using a group-theoretical approach, we demonstrate that these observations are results of magnetic field-induced morphic changes in the crystal symmetries through the Lorentz force exerted on the lattice ions. This study thus reveals a novel process of controlling phonon properties in a soft ionic lattice by a strong magnetic field.

# | Oral Session B



## Light Capture and Energy Conversion in Plasmonic-Polymeric Hybrids

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Plasmonic nanomaterials have absorption cross-sections exceeding other classes of materials but dephase quickly into their dielectric environment. In this work, plasmonic gold nanorods are hybridized with soft polymers that act as acceptors creating a hybrid nano-antenna reactor system. We seek to understand the dominating transfer pathways in single particle plasmonic-polymeric hybrid systems by using single particle spectroelectrochemistry. Hyperspectral dark-field spectroscopy was used to characterize the energy transfer efficiencies of single hybrid structures by recording the surface plasmon resonance energy linewidth change during *in situ* polymerization. The electrochemical polymerization was found to be selective and photoenhanced on the surface of the gold nanorods. We complement resonance energy transfer efficiencies calculated from single particle changes in linewidth with calculations from excitation polarization-dependent photoluminescence measurements. Non-radiative energy transfer efficiencies up to 50% are achieved in the plasmonic-polymeric hybrids. The understanding of interfacial transfer pathways between plasmonic-polymeric materials will lead to control and tunability of scalable hybrid nanoelectrodes.

## **Assembly of planar chiral enantiomers from achiral tetrahedra nanoparticles**

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Assembly of tetrahedra nanoparticles and understanding their packing behaviors have been extensively studied in both simulation and experiment for years. Despite the progress in mathematical construction of tetrahedra packings, only limited tetrahedra assemblies have been achieved by using semiconductor quantum dots, like quasi-crystalline phase and one-dimensional chain-like helical assemblies without translation features. Here, we demonstrated a new two-dimensional superlattice with planar helix structures by using uniform, large and sharp gold tetrahedra nanoparticles. Owing to the large size and sharp tips of tetrahedra, the tetrahedra nanoparticles adapted a rotation phase transition to offset the contacting area between each other to decrease the interparticle distance, which can reach to the length scale of interparticle interactions. Because of the existence of rotation phase transition, the formed enantiomers exhibit planar chiral features, which shows very promising applications in plasmonic chiroptics.

**Title: Efficient Photocatalytic PFOA Degradation Over Boron Nitride**

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Abstract: Per- and polyfluoroalkyl substances (PFAS), a group of persistent, pervasive, and toxic recalcitrant contaminants, were recently detected in drinking water supplies worldwide. The strong C-F bond makes them difficult to be degraded chemically or biologically, and so efficient water treatment technologies are urgently needed. I will describe the PFAS degradation abilities of hexagonal-phase boron nitride (hBN) in water with air as the oxidant, light (254 nm) as the energy source. Perfluorooctanoic acid (PFOA) was studied as the PFAS model compound. The mechanism insights of hBN, a widely recognized insulator, as a photocatalyst here will be discussed and the detailed catalytic reaction pathways of PFOA degradation over hBN will be proposed. Its applicability for other PFAS will be discussed.

## **Real-time Detection of Nitric Oxide using Photonic Microring Resonator in Physiological Medium**

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Nitric oxide (NO) is one of the most critical biomarkers involved in numerous physiological processes such as vasodilation, angiogenesis, neurotransmission, wound healing, immune response, *etc.* Thus, highly sensitive, robust, high spatiotemporal, and real-time monitoring of NO is of utmost importance. However, detection of NO in the physiological milieu is challenging due to its low concentration (pM-nM), short lifetime, small diffusion length, presence of other interference molecules, *etc.* Traditional detection methods are either indirect and suffer from low precision/sensitivity (Griess Assay) or require extensive sample preparation, complex instrumentation (Chemiluminescence, EPR) precluding real-time in vivo study. Electrochemical sensors, although very promising, are affected by EM interference and require a large surface area and longer polarization time. Here, we demonstrate an ultra-small photonic NO sensor using Si microring resonator (MRR) capable of real-time, continuous, high spatiotemporal detection of NO with sub-uM sensitivity. MRR is a resonant device that quantifies NO upon binding on sensor surface by resonance shift. The sensor is functionalized with hemin chloride to achieve high selectivity against potential interferents in the physiological medium. Its high sensitivity enables detection of NO released by stimulated RAW 264.7 macrophage cells demonstrating its practical functionality in a complex biological system. Therefore, we envision that this technique will pave the way for in vivo study to better understand NO's complex functionality and for therapeutic guidance.

## Synergistic plasmonic photocatalysis on Al-Pd-Fe trimetallic nanodisks

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Antenna-reactors are nanoparticle complexes consisting of a light-harvesting antenna combined with a specific type of catalytic reactive site. In plasmonic photocatalysis, antenna-reactor complexes can efficiently capture light energy to drive simple chemical reactions, such as H<sub>2</sub> dissociation or NH<sub>3</sub> decomposition. However, many important chemical transformations would actually need multiple reactors to catalyze different intermediate processes. Here we demonstrate precisely oriented planar Al-Pd-Fe trimetallic nanodisk trimers, employing Pd to catalyze D<sub>2</sub> and Fe to activate NH<sub>3</sub>. 45°, 90°, 180° trimers, and Al-Pd and Al-Fe dimers were fabricated to offer different relative positions between Pd and Fe reactors on a single Al “antenna” nanodisk. The NH<sub>3</sub>-D<sub>2</sub> exchange reaction can reach a maximum reaction rate when the ‘forced plasmon’ in an Fe nanodisk is excited with a Pd nanodisk in closest proximity (45° trimer). The reactivity on the Fe nanodisk reactor will be turned off once the Pd nanodisk is too far away from the Fe nanodisk (180° trimer). Combining hot carrier calculations and quantum mechanical reaction pathway theoretical analysis, we conclude that the hot carriers generated on Fe and the deuterium spillover from Pd are key to optimizing this reaction. This planar nanodisk geometry offers a modular system to understand the spatial dependence of antenna-reactor photoreactivity, with quantitative precision, and paves the way for the design and application of plasmonic antenna-reactor photocatalysts for substantially more complex chemical reactions.

# | Oral Session C

# Opening the Black Box: Examining Convolutional Neural Network Approximations of Quantum Spin Systems

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## Abstract

Integrating neural networks with Quantum Monte Carlo methods has become a popular choice for solving quantum physics problems. In this work, we open up the 'black box' to uncover how a convolutional neural network (CNN) successfully approximates the lowest energy states of a simple one dimensional spin chain. We further look at how the physics of our quantum system, such as symmetries, manifest in the CNN during training. We can use this connection to improve the training of our CNN and gain insight into why certain neural network architectures are well suited for certain physics problems.

**Title: Terahertz Magneto-optical Spectroscopy of  $\text{La}_{0.875}\text{Sr}_{0.125}\text{MnO}_3$** 

Fuyang Tay, Jiaming He, Nicolas Marquez Peraca, Xinwei Li, Andrey Baydin, Jianshi Zhou, and Junichiro Kono

Lanthanum strontium manganite ( $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  or LSMO) is one of the most complex strongly correlated materials, exhibiting a variety of phases. Depending on the composition ( $x$ ), temperature ( $T$ ), and magnetic field ( $B$ ), the nature of the system fundamentally varies, both electrically (metallic or insulating) and magnetically (paramagnetic or ferromagnetic). It is believed that there exists a strong interplay among the charge, spin, orbital, and lattice degrees of freedom, but a microscopic understanding has been elusive. In particular, it is not understood what causes the colossal magnetoresistance (CMR) effect at around the Curie temperature and the metal-insulator transition at low temperatures in underdoped LSMO ( $0.1 < x < 0.15$ ). Here we studied different phases of LSMO for  $x = 0.125$  as a function of temperature and magnetic field via terahertz (THz) time-domain magnetospectroscopy. Our optical conductivity spectra clearly revealed a THz CMR effect and indicated that the material is not governed by the Drude model even in the metallic phase. We observed a sudden jump in the THz dielectric constant when the temperature was cooled down through the magnetic ordering temperature. A jump in dielectric constant also occurred as a function of a magnetic field at a constant temperature. These observations provide significant new insights into the underlying mechanism of the various phase transitions that occur in LSMO at  $x = 0.125$ .



## **Dissipative Hot-spot Enabled Shock and Bounce Dynamics via Terahertz Quantum Quenches in Helical Edge States**

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### **Abstract**

We study quantum quenches of helical liquids with spin-flip inelastic scattering. Counterpropagating charge packets in helical edges can be created by an ultrashort electric pulse applied across a 2D topological insulator. Localized “hot spots” that form due to scattering enable two types of strongly nonlinear wave dynamics. First, propagating packets develop self-focusing shock fronts. Second, colliding packets with opposite charge can exhibit near-perfect retroreflection, despite strong dissipation. This leads to frequency doubling that could be detected experimentally from emitted terahertz radiation.

## Laser-Induced Fluorescence Imaging of a Magnetically Confined, Spin-Polarized Ultracold Neutral Plasma

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Ultracold neutral plasmas (UCNPs), created by photoionization of a cold gas, are an excellent platform for studying neutral plasmas in far more complex environments such as plasma in the Sun's atmosphere, white dwarf stars, and inertial-confinement fusion devices. Magnetized UCNPs are of current interest because of the interplay of magnetization and strong coupling, connection to plasma confinement, and modification of recombination dynamics in strong fields. We recently demonstrated the magnetic confinement of UCNPs at the null of a biconic cusp, or quadrupole magnetic field, with confinement times of up to 0.5 ms. Here, we describe our use of laser-induced fluorescence imaging of a magnetically confined UCNP to obtain spatially resolved measurements of ion density, hydrodynamic flow velocity, temperature, and spin polarization. Our observations demonstrate the ions are highly spin-polarized immediately after plasma creation, and the spin polarization is long-lived throughout plasma expansion and confinement.

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**Title:** Toward the studies of many-body phenomena with a trapped-ion quantum simulator

**Author:** Visal So (co-authors: R. Zhuravel, M. Sheffield, C. Liebenthal, and G. Pagano)

**Abstract:**

Trapped atomic ions are one of the leading platforms for the simulation of spin models. Here we present our progress on the construction of a multi-species trapping apparatus for Ytterbium and Barium ion chains. The system is based on a segmented four-blade Paul trap, which provides a large numerical aperture for high-resolution imaging ( $NA \sim 0.6$ ) and individual addressing ( $NA \sim 0.3$ ). The electrodes have been devised to optimize the homogeneity of the confinement radiofrequency field along the trap axis and to lower the required voltage to achieve quasi-uniformly spaced ion chains. We will also report our effort to extend this trap design to a monolithic three-dimensional trap with high precision electrode alignment utilizing laser writing and controlled glass etching techniques. By using internal electronic states within each ion to encode spin degrees of freedom and the normal phonon modes of the ion chain to tailor the interactions among the qubits, we aim to efficiently investigate spin Hamiltonians beyond the ability of classical computers. The apparatus is designed to give us precise control of both unitary and dissipative evolutions of the spin systems, allowing us access to new frontiers of quantum simulation, including the realization of quantum spin glass models and the study of lattice gauge theories.

# | Oral Session D

## **Al@TiO<sub>2</sub> Core-Shell Structures for Hot Carrier Photocatalysis**

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Plasmon-induced hot carriers have been demonstrated to facilitate photocatalytic processes. To effectively generate and utilize hot carriers, antenna-reactor heterostructures are developed by combining light-absorbing plasmon nanostructures and active surface catalytic materials. Here we introduce Al@TiO<sub>2</sub> core-shell nanoparticles of tunable thickness as photocatalytic antenna-reactors for hot electron-mediated H<sub>2</sub>/D<sub>2</sub> exchange and hot hole-mediated MeOH dehydration. During Al@TiO<sub>2</sub> synthesis, the insulating native oxide layer of Al nanocrystals which impedes the charge transfer pathway is removed and replaced by a semiconducting TiO<sub>2</sub> shell. 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 TiO<sub>2</sub> shell to promote chemical reactions. Furthermore, the TiO<sub>2</sub> layer imparts significantly enhanced aqueous stability to the Al nanocrystals, greatly increasing the range of potential reactions that these structures can be applied to. The Al@TiO<sub>2</sub> 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.

## Electron Transport through Nucleobase-Bonded Graphene Nanoribbon Junctions

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Carbon and hydrogen bonding constitute the backbone of life; in the form of graphene, possibly functionalized by DNA nucleobases, these hold promise for programmable assembly of graphene-based nanoelectronic devices. It is still unknown how hydrogen-bonded junctions inherent in such devices will perform as electron transport media. Here, we design nucleobase-bonded graphene nanoribbons and quantify their quantum transport characteristics using first principles calculations. Pronounced rectifying behavior and negative differential resistance are found, as well as high conductance of certain structures, with the guanine-cytosine junction in general being superior to other variants. The identified sensitivity of the current response to atomic details of the interfaces offers initial hints and guidance for experimental realization.

## Effective aspect ratio, phase behavior and macroscopic fiber properties of polydisperse, bimodal carbon nanotube solutions.

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Carbon nanotubes have the ability of strongly bundling together via Van Der Waals forces to form light weight macromaterials with high electrical, mechanical, and thermal properties. Consequently, there has been a great interest in developing wet spun CNT fibers, since their promising properties can be used in a wide variety of applications such as cabling, wearable electronics, biomedical applications, and energy applications. CNT fiber technology has improved dramatically over time. However, the spinning process needs to become more efficient to decrease the CNT fibers cost and environmental impact. The macroscopic properties of CNT fibers are dependent on the CNT aspect ratio and phase behavior. The phase behavior of CNTs is well described by CNT aspect ratio, such that the isotropic-to-nematic phase transition behaves accordingly to Onsager's classical theory for rigid rods. In this work, we study the effect of CNT length and diameter polydispersity on the aspect ratio, the phase behavior, and the macroscopic electrical and mechanical properties of CNT fibers. The effect of high polydispersity in CNT solutions has not been previously reported and it is not yet fully understood.

Two types of CNTs, high aspect ratio (rod length divided by rod diameter  $L/D$ ) CNTs and low aspect ratio are mixed in different weight fractions. Transmission electron microscopy, cross-polarized optical microscopy, and extensional rheometry to characterize the phase behavior and viscosity-averaged effective aspect ratio of these bimodal CNT solutions. Finally, CNT fibers are spun via wet spinning to determine their macroscopic electrical and mechanical properties. The results show how the fraction of long-to-short tubes in solution affect the isotropic-to-nematic phase transition and the solution effective aspect ratio as determined by capillary thinning extensional viscosity measurements. These predictions are key to better understand and optimize the properties of macroscopic CNT materials made from polydisperse solutions at high concentrations.

## Maximizing and minimizing the boundary scattering mean free path in diameter-modulated coaxial cylindrical nanowires

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### ABSTRACT

The thermal conductivity ( $k$ ) of semiconducting nanomaterials is influenced by the geometry-dependent phonon boundary scattering mean free path ( $\Lambda_{\text{Bdy}}$ ). Although prior work has calculated  $\Lambda_{\text{Bdy}}$  of periodically corrugated rectangular nanowires and used these results to study phonon backscattering in nanomaterials,  $\Lambda_{\text{Bdy}}$  remains unknown for recently fabricated periodic coaxial cylindrical nanowires. Here, we use phonon ray tracing simulations to comprehensively study the effect of geometric parameters on  $\Lambda_{\text{Bdy}}$  in coaxial cylindrical nanowires. We find that for a fixed smaller cylinder diameter ( $D_1$ ) and cylinder length ratio,  $\Lambda_{\text{Bdy}}$  of periodic nanowires can be maximized or minimized via geometric control of the pitch ( $p$ ) and larger cylinder diameter ( $D_2$ ). Our simulations show that saturated phonon backscattering for small pitch ratio ( $p_r$ ) nanowires gives rise to a minimum in  $\Lambda_{\text{Bdy}}/D_1$  at  $p_r$  near unity, while the maximum in  $\Lambda_{\text{Bdy}}/D_1$  for large  $p_r$  nanowires can be understood using a simple thermal resistor model for two individual nanowires in series. Combining our  $\Lambda_{\text{Bdy}}$  calculations with analytical phonon dispersion and bulk scattering models, we predict that  $k$  of periodic silicon nanowires with fixed  $D_1$  can be tuned by up to 34% in the boundary scattering dominated regime by modifying  $D_2$  and  $p$ , and that variations as large as 135% can be observed in the normalized thermal conductance. Our results provide insight into geometry-dependent phonon backscattering and can be used to predict  $k$  of periodic cylindrical nanowires over a range of temperatures and geometric lengthscales.



**Title:** Single-Cell Stochastic Modeling of the Action of Antimicrobial Peptides on Bacteria

**Authors and affiliation**

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**ABSTRACT**

Antimicrobial peptides (AMPs) produced by multi-cellular organisms as their immune system's defense against microbes are actively considered natural alternatives to conventional antibiotics. Although substantial progress has been achieved in studying the AMPs, the microscopic mechanisms of their functioning remain poorly understood. Here, we develop a new theoretical framework to investigate how the AMPs are able to neutralize the bacteria efficiently. In our minimal theoretical model, the most relevant processes, AMPs entering and the following inhibition of the single bacterial cell, are described stochastically. Using complementary master equations approaches, all relevant features of bacteria clearance dynamics by AMPs, such as the probability of inhibition and the mean times before the clearance, are explicitly evaluated. It is found that both processes, entering and inhibition, are equally important for the efficient functioning of AMPs. Our theoretical method naturally explains a wide spectrum of efficiencies of existing AMPs and their heterogeneity at the single-cell level. Theoretical calculations are also consistent with existing single-cell measurements. Thus, the presented theoretical approachclarifies some microscopic aspects of the action of AMPs on bacteria.

# | Graduate Student | Posters

# Single-Particle Hyperspectral Imaging Reveals Kinetics of Silver Ion Leaching from Alloy Nanoparticles

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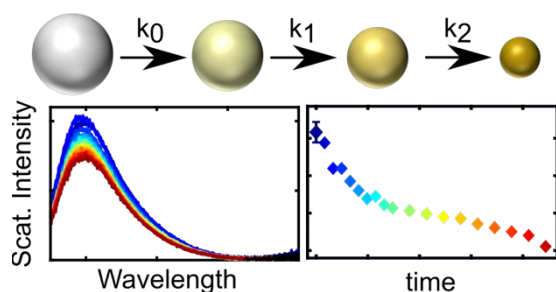
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Gold-silver alloy nanoparticles have attracted attention for multiple applications, including heterogeneous catalysis, optical sensing, and antimicrobial properties. The inert element gold can act as a stabilizer for silver to prevent particle corrosion to slow down silver ion leaching and increase the durability of plasmonic alloy nanoparticles in sensing or catalytic applications. On the other hand, intentional release of antimicrobial silver ions has been used to fight infections caused by bacteria. Understanding silver ion leaching from gold-silver alloy nanoparticles is a therefore prerequisite to designing alloy nanoparticles with either unintended or intended corrosion. However, little is known about the mechanism and kinetics of silver ion leaching from bimetallic gold-silver nanoparticles and how it is correlated with particle size and silver content, especially not on a single-particle level. To characterize the kinetics of silver ion release from gold-silver alloy nanoparticles, we employed a combination of electron microscopy and single-particle hyperspectral imaging with an acquisition speed fast enough to capture silver ion leaching for a statistically relevant number of individual nanoparticles. Our studies confirmed a reduction in corrosion rate due to the alloying with as little as 10-20 mole% gold. Single-particle leaching profiles revealed two leaching stages, with a large heterogeneity in rate constants. We modelled the initial leaching stage with a shrinking-particle model with a rate constant that exponentially depends on the silver mole fraction. The second, slower leaching stage is controlled by diffusion of silver atoms through a passivating gold rich lattice, and a change in electrochemical potential of the nanoparticle. Individual nanoparticles with similar sizes and compositions exhibited completely different dealloying yields. Most nanoparticles released silver completely, but 25% of them appeared to arrest corrosion. Calculations of average size together with SEM revealed that nanoparticles became slightly porous. Our findings suggest that alloy nanoparticles, produced by scalable laser ablation in liquid, together with kinetic studies of silver ion leaching, provide an approach to selectively design the durability or anti-microbial bioactivity of alloy nanoparticles.



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The authors declare no competing financial interest.

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## **Effect of the roughness of self-assembled monolayers on protein dynamic at a reversed-phase chromatographic interface**

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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, also called biologics. One of the most widely used methods of protein purification and separation is chromatography. Despite the wide industrial usage and intensive development, 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 biologics, 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 reversed-phase chromatography which separates proteins based on their hydrophobicity. In this work, single-molecule fluorescence microscopy is utilized to reveal the details of adsorption-desorption dynamics of  $\alpha$ -lactalbumin, a well-studied model protein, at the interface of C18 bonded silica – the most popular stationary phase for reversed-phase chromatography. Based on the difference of  $\alpha$ -lactalbumin transport on the surface, single-molecule tracking uncovers two types of protein population: continuous-time random walk and immobile populations. By changing C18 coverage of the surface it was possible to tune the prevalence of each population. Characterization techniques such as atomic force microscopy and contact angle helped explain observed single-molecule results through hydrophobicity and surface roughness changes.

## **Aligned Carbon Nanotubes Films and Their Applications as a Thermal Emitter**

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Single walled carbon nanotubes (SWCNTs) is among the leading materials proposed to serve as thermal emitters within thermophotovoltaic reactors. SWCNT's proposed use stems from its extreme anisotropy, being conductive along the axis of the nanotube, and dielectric everywhere else. This anisotropy results in a hyperbolic isofrequency contour, allowing SWCNT to support a much wider array of wave vectors than what can propagate in free space- at the cost of free space light not coupling directly to SWCNT without the introduction of a metasurface. In this work, we calculate, via the finite element method, the absorption of a SWCNT film with a periodic diffraction grating etched into it, noting enhancements from both a direct coupling to CNT, and from the formation of indefinite cavity modes within the diffraction grating. We demonstrate that, by optimizing the topology of the diffraction grating to maximize these two effects, greater absorption over a wider frequency range can be reached than what either of these effects could produce alone. Our work reinforces SWCNT's potential as a thermal emitter and informs manufacturers of the optimal ways to introduce SWCNT films into thermophotovoltaic reactors.

**Title:** Adiabatic initiation of the CuO/Al thermite reaction via micro-particle impact

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**Abstract:** Mechanical ignition of thermite reactions remains poorly understood because of experimental difficulties with assessing reaction pathways at microstructural length-scales under well-defined loading conditions. The present work overcomes this obstacle using small-scale impact experiments and complementary hydrocode simulations, which together enable characterization of the Al/CuO thermite reaction at an isolated heterophase interface. Laser-induced particle impact testing is used to launch single micron-scale CuO particles at an aluminum target at speeds in the range 100 to 1100 m/s. *In situ* observations show a clear transition from particle rebound to penetration with increasing striking velocity. In the rebound regime, there is no evidence of reaction, despite contact times of ~200 ns, an order of magnitude longer than the reaction timescales reported in previous studies of mechanical ignition in this materials system. By contrast, post-mortem characterization of a CuO particle that penetrated the Al target reveals a 20 nm thick nanocrystalline reaction layer comprising metallic Cu,  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>, and metastable  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>. The thickness of this reaction layer matches that of a molten Al interfacial layer observed in hydrocode simulations of the same particle impact. Heat transport considerations show that the reaction layer forms in 10's of nanoseconds, in line with timescales reported for conventional shock-induced thermite reactions. These results indicate that local melting via adiabatic deformation drives mechanical ignition of thermite reactions, establishing an important connection between thermal ignition under high heating rates and mechanical ignition.

## Nonlinear Vacuum Ultraviolet Metalens

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Vacuum ultraviolet (VUV) light has become an integral part of science and technology such as molecular spectroscopy, nanolithography and biomedical procedures. Next-generation VUV technology requires nanoscale VUV light generating devices, however few materials offer low-loss solutions within this wavelength range. We demonstrate a nanophotonic metalens, which focuses VUV light generated by the nonlinear optical process of second harmonic generation. An array of 150nm zinc oxide nanoresonators compose the 150nm thick metalens and convert incident 394nm radiation into focused 197nm VUV light with a spot diameter of 1.7  $\mu\text{m}$  and a 21 times power density enhancement. The ultracompact design results in a phase-matching free VUV source, which may be integrated to streamline VUV systems. This work provides a platform for developing low loss multifunctional VUV components, increasing the accessibility of the VUV regime.



## Towards 3-Dimensional Optical Lattice for Ultracold Strontium

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An optical lattice is a periodic potential created by standing EM waves resulting from pairs of counterpropagating laser beams. Optical lattices can be a powerful tool for quantum simulation of many body physics. Here, the development of a two-dimensional (2D) optical lattice to be used to create arrays of 1D tube-shaped micro traps for studies of 1D quantum gases is described. A 1064 nm fiber amplified laser system is used to create two orthogonal pairs of standing waves that together form a 2D lattice. By delivering 4W of power to each arm of the lattice and focusing the beams to a beam radius of ~250 microns at the location of the atoms, we create a 2D lattice with a maximum trap depth of 70 times the photon recoil energy. The trap depth vs. light power of the lattice is simulated numerically with code and characterized experimentally using Kapitza-Dirac diffraction. With tunable trap depth, this lattice will allow preparation of 1D atom samples with a range of different average interaction energies thereby providing a rich yet simple system to study. Initial experiments will use Rydberg-molecule spectroscopy to probe the non-local spatial correlation function of the 1D quantum gases with different interaction strengths. Later down the path, we hope to tune the interaction strength to study exotic phases like the Tonks-Girardeau gas in 1D quantum gas.

# Non-Hermitian metasurfaces with non-trivial topology

## SCI Summer Research Colloquium 2021

Ciril Samuel Prasad, Frank Yang, Alex Y.Hwang, Chloe Doiron, and Gururaj V. Naik

July 30, 2021

### Abstract

Non-Hermitian and topological photonics have been the subject of intense research in recent years due to numerous exotic physical effects observed in such systems [2, 3]. However, their implementation in nanophotonics is challenging due to poor confinement of light at deep-subwavelength scales. Here, we overcome the limitation to experimentally demonstrate a non-Hermitian metasurface with nontrivial topology in the  $k$ -space [1]. Our hybrid plasmonic-photonic system exhibits an exceptional concentric ring with Z3 topology. This demonstration unlocks quantum many body phenomena in nanophotonics and paves the way towards unconventional light sources at nanoscale.

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## Surface Modification, Biostability, and Cytotoxicity of Size- and Shape-controlled Aluminum Nanocrystals

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Aluminum (Al) is a cost-effective, Earth-abundant metal that is widely used in day-to-day consumer applications. Despite the ubiquitous use of Al-based materials, little work has evaluated the potential of Al nanoparticles (NPs) in biomedical and environmental applications due to the lack of synthetic control over Al NPs size, shape, and surface chemistry. Recent developments in our lab have enabled synthesis of precisely size- and shape-controlled Al nanocrystals (Al NCs) that possess a 3-5 nm oxide layer and tunable plasmon resonances spanning the UV and visible regions. Here, we aim to functionalize Al NCs of variable size and evaluate their aqueous stability and cytotoxicity, with hopes of understanding the biomedical and environmental impact of tunable nanoscale Al. We have functionalized Al NCs with silane-terminated poly(ethylene glycol) of various molecular weights and human serum albumin. Optical properties and physical characteristics, as well as particle stability in milli-q water and at physiological conditions, have been investigated for bare and functionalized Al NCs. The cytotoxicity of bare Al NCs as a function of particle diameter has been studied in *E. coli*. Our results indicate that bare Al NCs do not cause appreciable cell death in *E. coli* at 100  $\mu\text{g/mL}$ , regardless of size, and that functionalization of Al NCs increases water solubility without hindering degradation in aqueous media. These findings suggest that Al NCs are a promising low-cost and biodegradable alternative to gold and silver nanoparticles in biomedical and environmental applications.

## Colloidal Synthesis of 1D Anisotropic Aluminum Nanostructures for Plasmonic Applications

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Anisotropic nanostructures have been shown to be key contributors for a variety of next generation electronic, optical, energetic, and biochemical devices, but many of them rely on elementally scarce noble metals. One emerging alternative, Al, has been proposed due to its relative elemental abundance, and we have demonstrated growth of several 3D nanocrystals with faceting analogous to traditional Au and Ag shapes. Recent Al nanocrystal advances have resulted in increased understanding of size, shape control, and the growth mechanisms to achieve both. Here we demonstrate an adaptation of noble metallic kinetic growth principles to yield colloidal 1D Al nanostructures. By reducing the generation of elemental Al atoms during constrained growth, we kinetically force addition along one or two axial directions, leading to nanobars and nanowires. We accomplish this through modification of the catalyst, a factor currently unique to Al nanocrystal synthesis, to slow the reduction of  $\text{AlH}_3$ . This approach allows for the ability to fine tune the reaction landscape of nanocrystal growth, yielding a chemical syntheses of highly anisotropic Al nanostructures. Furthermore, we apply the colloidal nanowires as plasmonic waveguides, showcasing their relative stability at guiding light when compared to contemporary noble metal options. This work demonstrates a new avenue of research for Al nanocrystal synthesis and presents an atmospherically stable material for ultraviolet and visible waveguiding.

**Title: Study of hydrophobicity dependence of protein dynamics in stimuli-responsive hydrogels with 3D single molecule tracking**

**Author:** Dongyu Fan

**Abstract**

Stimuli-responsive hydrogels that respond to external triggers have promising applications in protein separation. The understanding of protein interactions with such hydrogels are limited by previous ensemble level studies that failed to address heterogeneity which is essential for optimizing separation processes. In this work, 3D single molecule tracking is applied to determine the dynamics of a model protein, lysozyme, in thermo-responsive hydrogels poly(N-isopropylacrylamide) (PNIPAm). Results indicate that the adsorption rate of lysozyme is controlled by hydrogel hydrophobicity, with a higher adsorption rate when the temperature is higher than PNIPAm's lowest critical solution temperature (LCST) at 32°C. The residence time of lysozyme on hydrogel is controlled by mesh sizes of the hydrogel network that's altered by thermo-responsive phase change. This work establishes the relationship between hydrogel structure and surface properties to protein transport mechanisms.

## **Characterizing Evolutionary and Physical Energy Landscapes of Evolving, Devolving, and Random Sequences**

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Proteins are the essential machinery of every cell and are encoded by sequences energetically distinct from random assortments of amino acids. Due to evolutionary constraints, protein sequences cooperatively fold into unique, energetically minimized three-dimensional structures in timescales as short as microseconds. The importance of maintaining the stable protein structure according to evolution can be quantified by the selection temperature. The selection temperature can be calculated using coarse-grained free energy functions, and protein-specific information theoretic Hamiltonians utilizing genomic data. Previous studies have found selection temperatures to be below physiological protein folding temperatures, indicating that energetically minimized structures are an important evolutionary constraint. Our work studied a broader array of proteins than previously surveyed. We found that proteins' selection temperatures in the study are below physiological temperatures, indicating that folding energetics are an important evolutionary consideration for a wide range of proteins with various biological roles.

Furthermore, we incorporated temporal information from the evolutionary process by studying formerly protein-coding genes randomly mutated over time called pseudogenes. We characterized the energies of sequences at differing stages of devolution and evolutionary pressure, and found that devolving pseudogenes modified by mutations over time can be energetically distinguished from protein sequences.

## **Understanding the Nature of the Photothermal Signal in the Small and Large Particle Limits**

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In recent decades photothermal microscopy has been utilized to explore the absorption properties of a wide variety of materials, such as plasmonic nanoparticles, independent of scattering. This technique utilizes two different laser sources: a pump beam that resonantly excites and heats the target sample embedded in a liquid medium, and a probe beam that is scattered by the change in refractive index of the liquid medium upon sample heating. Theoretical models have been developed alongside extensive experimental evidence to interpret the nature of the photothermal signal. However the models developed thus far have only been applied to systems in the small particle limit that do not possess their own intrinsic scatter resonances, and thus scattering contributions from the target system itself to the photothermal signal have been assumed to be negligible. Working in collaboration with researchers at the University of Washington and Temple University, we have developed a new theoretical model that incorporates systems in the large particle limit with intrinsic scattering resonances and the influence that it has on the resulting photothermal signal, with experimental evidence that corroborates the validity of the model.

## Machine-Learned Decision Trees for Predicting Gold Nanorod Sizes from Spectra

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Electron microscopy is often required in order to precisely correlate the size and shape of plasmonic nanoparticles with their optical properties. Eliminating the need for electron microscopy is one crucial step towards *in situ* sensing applications, especially for complicated sample conditions such as during irreversible chemical reactions or when particles are embedded in a matrix. Here, we show that a machine learning decision tree can accurately predict gold nanorod dimensions over a wide range of aspect ratios. The model is trained using ~400 nanorod geometries and corresponding scattering spectra obtained from finite-difference time-domain simulations. We test the model using a set of experimental spectra and sizes obtained from correlated scanning electron microscopy images, resulting in estimates of small and large nanorods dimensions within a relative error of 10%. Analysis of the decision tree structure reveals that a simple correlation with resonance energy and linewidth of the localized surface plasmon resonance is sufficient to predict nanorod dimensions, notably outperforming more complicated models. Our findings illustrate the advantages of using simple machine learning models to infer single particle structural features from their optical spectra.



**Title: Imaging Exosomes by Cryo-Electron Microscopy****Abstract:**

Nanosized exosomes are type of extracellular vesicles that are produced by all known organisms and play an important role in cell-cell communication and physiology. We have observed morphological diversity when we purified exosomes from tumorigenic and non-tumorigenic cell lines. However, a detailed morphological analysis has never been performed on exosomes purified by various isolation techniques. In this study, we were able to classify exosomes into seven different categories according to their shape using cryo-electron microscopy. Motivated by these findings we want to next utilize engineered exosomes with siRNA incorporated within their lumen and perform 3D reconstruction on these engineered exosomes. We have developed a GMP-grade process to generate exosomes embedded with siRNA that are currently being used for clinical trials in pancreatic cancer patients. By imaging the clinical-grade exosomes we will help the exosomes research field to widen their understanding of the structure of exosomes as well as make sure there is no batch-to-batch variability for the clinical grade exosomes.

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## Spectroscopic Titration Shows (n,m)-Dependent Displacement of SDS by ssDNA on Single-Wall Carbon Nanotubes

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Single-stranded DNA oligonucleotides (ssDNA) are uniquely customizable polymers that are useful for coating, suspending, and structurally sorting single-wall carbon nanotubes (SWCNTs) in water. However, SWCNT dispersions are instead commonly prepared using inexpensive amphiphilic surfactants such as SDS. By monitoring changes in the nanotube fluorescence wavelengths and intensities, we show that such SDS coatings on dispersed SWCNTs can be controllably displaced by the addition of small amounts of ssDNA. The displacement data can be well represented by kinetic modeling, giving the time scales for equilibration of the coating composition. We measured spectra of SWCNT samples that were dispersed in low concentrations of SDS, then treated with small amounts of ssDNA and allowed to reach equilibrium. Plots of the final spectral shifts as a function of added ssDNA provide (n,m)-specific “titration” curves that show strongly diameter-dependent behavior. Smaller diameter nanotubes undergo SDS displacement at the lowest ssDNA concentrations. The limiting spectral shifts suggest that SWCNT surfaces become coated with adsorbed SDS as well as ssDNA. We will also illustrate how the (n,m)-dependent displacements found here can be used for structural sorting of mixed SWCNT samples.

## Plasmon-Mediated Generation of Solvated Electrons for Chemical Transformations

Kyle D. Chapkin,<sup>1,3</sup> David Solti,<sup>1,2</sup> David Renard,<sup>1,2</sup> Aaron I. Bayles,<sup>1,2</sup> Benjamin D. Clark,<sup>1,2</sup> Gang Wu,<sup>4</sup> Ah-Lin Tsai,<sup>4</sup> and Naomi J. Halas<sup>1,2,3,5</sup>

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Solvated electrons are free, unbound electrons delocalized within a solvent cage and are among the most reductive single species available for redox and radical reactions. Until recently, the predominant methods for generating solvated electrons have focused on relatively destructive and uncontrolled techniques, either requiring high-energy electrons or photons to temporarily form free electrons in solvent clusters, or bulk dissolution of an alkali earth metal to act as a constant electron donor. None of these options allow for solvated electron use in precise and sensitive chemical reactions. Herein, we have developed a method for generating solvated electrons in a non-destructive and controlled manner, through the excitation of the localized surface plasmon resonance (LSPR) of aluminum nanoparticles with visible light. We characterized the solvated electrons generated through electron paramagnetic resonance (EPR) and ultrafast transient absorption (TA) spectroscopy, and confirmed they matched those reported in the literature. Furthermore, a simple organic transformation was performed *in situ* to demonstrate the applicability of this technique as a platform for organic chemists. This system offers a simple, non-destructive, light-directed framework for experimentalists to utilize, without the drawbacks of past solvated electron generation methods.

## **Streamlined identification of PAHs/PACs in environmental samples using ultracompact spectroscopy platforms and machine learning strategies**

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Polyaromatic hydrocarbons (PAHs) and their functionalized derivatives are ubiquitous environmental contaminants with carcinogenic, mutagenic, and teratogenic human health effects. Current gold standard methods of identification of polyaromatic hydrocarbons are costly, time-consuming, and not portable. To overcome these challenges, we couple Surface-Enhanced Raman spectroscopy with machine learning for the portable ultrasensitive sensing and identification of PAHs in complex mixtures. Surface-Enhanced Raman spectra of mixtures of PAHs were collected and analyzed using independent component analysis. Surface-Enhanced Raman spectra of each PAH present in the complex mixtures were reconstructed using independent component analysis. This result demonstrates the ability of Surface-Enhanced Raman spectroscopy coupled with machine learning to computationally separate PAH mixtures.

## Photodecomposition of 2-CEES on Al Nanoparticles

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2-chloroethyl ethyl sulfide (2-CEES) is a surrogate of the chemical warfare agent (CWA) sulfur mustard whose decontamination has been investigated for decades. However, these decompositions are usually based on thermocatalysis, which limits their applications given that heat sources are generally less portable and slow in response. Recent developments in the diode laser industries give rise to portable laser sources with low dead volume and quick response, allowing for flexible light-induced chemistry. In this work, the photodecomposition of 2-CEES is studied using Al Nanoparticles (NPs). Combining the plasmonic Al core with the self-restricted alumina surface as the reaction substrate, the photodecomposition of 2-CEES on the Al NPs was performed with high efficiency. The alumina surface can absorb the HCl product effectively to prevent secondary pollution, with the S physically adsorbed in the form of thioethers or thiols. These Al NPs can be regenerated simply by annealing in He. The effect of different surface pretreatment on the reactivity of the photodecomposition was also investigated, where vacuum-pretreated and NH<sub>3</sub>-pretreated samples showed higher reactivity.

## Controlling the acoustic vibrations of single lithographic nanoparticles through the substrate binding strength

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Acoustic vibrations of plasmonic nanoparticles provide unique insight into the mechanical properties of the particles and are promising for sensing applications. The vibrational behavior can be monitored through all-optical means, allowing contact-free measurements of objects on the nanoscale. Electron-beam lithography provides a favorable fabrication method of substrate-based nanoparticles for sensing applications, as it offers great control of particle shape and size. However, these lithographic nanomaterials exhibit short acoustic lifetimes due to intrinsic and extrinsic damping mechanisms, leading to small vibrational quality factors ( $Q$ ). Despite previous research efforts, there is still no clear picture of the relative contributions of extrinsic versus intrinsic effects to the overall damping. Here, we utilize single particle transient extinction spectroscopy to study the vibrational behavior of gold nanodisks on glass and sapphire substrates in dependence of the particle-substrate binding strength. We experimentally and theoretically find that strong particle-substrate binding of gold nanodisks on glass, accomplished through thickened titanium adhesion layers, causes the creation of new acoustic modes that can exhibit strongly enhanced  $Q$  due to decreased extrinsic damping. Based on simulations, we observe that the occurrence and strength of this effect depends on the mechanical properties of particle and substrate and identify the relevant parameters. Finally, we suggest that the relative contributions of extrinsic and intrinsic damping to the overall damping depend on the binding strength between particle and substrate, with extrinsic and intrinsic parts dominating for strong and weak binding, respectively.

# Quenching of SWCNT Fluorescence by Rose Bengal Provides Insight about The Structure of Carbon Nanotube's Coating.

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Single-walled carbon nanotubes (SWCNTs) have attracted a great deal of attention during the past two decades because of their unique optoelectronic properties and their potential theranostics as well as nanoelectronics applications. One major impediment in the widescale use of carbon nanotubes is the heterogeneity of the as-synthesized SWCNT samples. One approach to solve this problem is by sorting different nanotube species based on the minuscule difference in their physical and chemical properties. One such a property that has been utilized to sort different chiralities of nanotube is the differential interaction of nanotubes with the dispersing agent.<sup>1,2</sup> Therefore, exploring the interaction of each individual carbon nanotube species with different dispersing agent, would have implications for sorting applications.

In this work we describe the charge transfer process between Rose Bengal dye molecule and SWCNTs, resulting in the p-doping and subsequent fluorescence quenching of the SWCNT species. The quenching showed a dependence on the structure of the surfactant around the nanotubes and therefore is used to study the coating of each SWCNT chirality by different dispersing agent.

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## Thermal Oscillators and potential synchronization properties

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Oscillators appear in many natural and technological systems, from pendulums to electric circuits. This poster describes a light irradiated thermal systems featuring countercurrent fluid channels acting as flow-driven thermal oscillators. In the context of light-harvesting for decentralized thermal energy storage systems, understanding oscillation and synchronization mechanisms in thermal oscillator arrays is crucial to improve storage efficiency and control heat release on-demand. Here, we first show how properly designed photo-thermo-fluidic modules exhibit the essential properties of harmonic oscillators, such as resonance condition and decay time. Furthermore, we study flow-driven thermal oscillators coupling, showing how two different oscillators can exchange thermal energy. Preliminary numerical results suggest the potential of synchronization between coupled thermal oscillators. Our current approach is based on tuning the interaction between two oscillators by reducing or increasing the amount of heat they exchange. Series and parallel configurations are investigated, showing peculiar anti-phase or in-phase heat trajectories. In the near future, we plan to define phase-locking and additional sync properties for thermal oscillators. The possibility to manipulate the synchronization properties of thermal oscillators will enable us to design optimized arrays and scale up the overall thermal storage capacity.



## **Geminal models for challenging electronic structure problems**

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Traditional quantum many-electron methods use one-electron functions called molecular orbitals as the building blocks of the wave function. Although these methods have many excellent features, they are not optimal for cases where two-body interactions become dominant. Wave function methods based on geminals or electron-pair building blocks might be better suited for these kinds of problems while being conceptually appealing due to their connection with chemical bonds. We discuss the challenges of replacing molecular orbitals with geminals and our recent progress in addressing them. We also present numerical evidence that the newly introduced geminal models accurately describe strong pairing interactions with a model Hamiltonian.

## **Strongly Interacting Two-component Coupled Bose Gas in 1D Optical Lattice**

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We study one-dimensional strongly interacting two-component bosons in an optical lattice with tunable same-site and nearest neighboring sites intercomponent coupling. Previous work studying two-component Bose–Hubbard model in deep Mott regime without consideration of coupling shows  $z$  anti-ferromagnetic and  $x$ - $y$  ferromagnetic spin phases in spin-1/2 (New J. Phys. 5 113, 2003) and Mott and  $x$ - $y$  ferromagnetic spin phases in spin-1 (Phys. Rev. A 92, 041602(R), 2015). Such a system is experimentally realizable as two component bosons (envisioned as two internal levels of an atom) in a tilted optical lattice. We introduce couplings via nearly resonant microwave field, and the intra-component tunnelings via light-assisted Raman transition. Coupling of the components substantially alters the previously observed spin phases revealing fascinating non-trivial spin correlations. The present consideration of inter-component coupling for unit occupancy gives rise to novel effective ordering of the spins leading to unprecedented spin phases: site-dependent  $z$ - $x$  spin configuration with tunable (by hopping parameter) proclivity of spin alignment along  $z$ . The examination goes beyond the mean-field approximation by employing exact analysis and Variational Monte Carlo with stochastic minimization on Entangled Plaquette states (EPS). The possibility of the exotic spin phases persisting at occupancy greater than unity and with complex intra-component tunnelings and inter-component coupling are discussed.

**Title:**

Dynamical Fermionization in Quenched One Dimensional Quantum Gases

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**Abstract:**

One dimensional systems in physics benefit from the enhancement of quantum mechanical effects in lower dimensions, leading to unique phenomena. An example of such a uniquely quantum and 1D phenomenon is dynamical fermionization. This occurs when strongly interacting 1D bosonic gases, initially confined in a harmonic trap, expand to asymptotically mimic the density profiles of fermionic gases. We discuss our demonstration of this phenomenon in spin gases, and the implications of this result for studying quantum dynamics and statistics.

# Electron-phonon coupling between TMDCs and substrates revealed by THz-induced SHG spectroscopy

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Coherent phonon control is a promising way to manipulate lattices and properties of two-dimensional (2D) materials. It can drive the atoms in crystalline lattice to much larger amplitudes than other conventional methods. However, this requires a comprehensive understanding of phonons and their interaction with electrons, etc. The interaction between 2D materials and substrates is of great importance since the properties of 2D materials are sensitive to substrates. Here we present a study of electron-phonon coupling between transition metal dichalcogenides (TMDCs) and substrates utilizing THz-induced second-harmonic generation (SHG) spectroscopy. In this work, we use intense THz pulse to excite a large population of phonons and measure their modulation of SHG signal. The observed unique optical nonlinearity suggesting extraordinary electron-phonon coupling between substrate and TMDCs. Further investigation demonstrates that this coupling is attributed to a new surface phonon mode of sapphire. This observation could not only advance our fundamental knowledge of the materials, but also open up new ways to enhance optical nonlinearity in 2D materials using different phonon frequencies in substrates.

## Mechanistic Study of Oxygen Doping of Single-Wall Carbon Nanotubes using Hypochlorite

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Single-wall carbon nanotubes (SWCNTs) are one-dimensional cylindrical structures that resemble a rolled-up graphene sheet. These artificial nanomaterials are fascinating because of the many interesting properties they possess, such as their electronic, optical, and physical features. With these properties in mind, chemically induced defects along the sidewalls of single-wall carbon nanotubes are a topic of great current interest. These chemical modifications have the potential to affect optical transitions in a way that can shift semiconducting fluorescence emission further into the near-infrared region. These shifts can be valuable in bio-imaging applications. Here we present further studies on the use of photoexcited hypochlorite ions as a reactant to produce oxygen-doped SWCNTs. Our studies focus on the effects of excluding dissolved oxygen during the reaction. We find greatly increased reaction rates and the appearance of additional shifted emission bands. These results, combined with kinetic data and quantum computations, provide insight into the doping mechanism. This work will enable more efficient and controlled production of carbon nanotubes with tailored optical properties.

## Finite element modeling of thermal oscillators for increased solar desalination efficiency

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A severe lack of access to fresh water endangers the health, food security, and industrial practices of billions of people around the globe. With climate change promising to exacerbate water scarcity in the coming decades, it is imperative to find clean energy solutions to increase water access efficiently and sustainably. Leveraging both renewable solar power and the Earth's immense salt water resources, evaporation-based desalination techniques have key advantages in terms of accessibility and scalability over conventional, heavy infrastructure-based desalination practices like reverse osmosis. However, despite the possibility of relieving water insecurity via inexpensive and modular solar purification systems, the efficiency of evaporation-based desalination is limited for practical use by the large energy demands dictated by the enthalpy of vaporization. A novel thermal desalination oscillator system, which combines nanophotonics-enabled solar membrane distillation with heat exchange between saline and distilled water streams of matched flow rate, recently showed significant gains in fresh water production at the system's resonance condition. This system, which is optimized by controlling flow rates as a function of incident sunlight intensity and further enhanced by a between-channel metal heat exchanger, is a particular case of a flow-driven oscillator, a recently discovered resonant oscillator driven by thermal-energy exchange and countercurrent mass flows instead of time oscillating signals. The thermal desalination oscillator has shown promise in improving solar desalination efficiency by exploiting this resonant behavior, though much work remains in further increasing heat transfer across the flow channels and eliminating bottlenecks like environmental losses and the low thermal conductivity of water compared to the previously aluminum or copper heat exchanger material. We use the finite element method to model real-world thermal desalination oscillators and explore novel configurations and corrosion resistant materials for heat exchangers which optimize heat transfer and distillate flux in resonant solar desalination systems. Our models additionally enable us to iterate upon prior nanophotonics-enabled membrane desalination designs and investigate further, much-needed environmental loss mitigation in thermal oscillators for maximal distillation efficiency. With our finite element modeling of thermal oscillators, we aim to provide new insight into the design of off-grid, cost-effective water purification technologies.

## Sustainable plasmonic photocatalysis

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Plasmonic photocatalysis enables an efficient conversion of light energy to chemical energy, which relies on noble metals as the catalyst. However, global reserves of noble metals are scarce, urging us to develop efficient, stable, and selective catalysts based on earth-abundant elements. In this work, we developed an earth-abundant photocatalyst for ammonia decomposition, showing a  $\sim 10^3$ -time enhancement of reactivity compared to its thermocatalytic rate. Hot carrier drives the reaction in the excited states, resulting in a smaller barrier and smaller surface coverages than the ground-state thermocatalysis.

In nitrous oxide decomposition reaction, hot carrier is demonstrated to improve the stability of the same catalyst which suffers from oxidation in thermocatalysis. These intrinsic advantages foresee the broader application of plasmonics photocatalysis in sustainable energy infrastructure.

**Towards Scalable Plasmonic Fano-Resonant Metasurfaces for Colorimetric Sensing**

*Benjamin Cerjan, Burak Gerislioglu, Stephan Link, Peter Nordlander, Naomi J. Halas\*, Mark H. Griep*

Transitioning plasmonic metasurfaces into practical, low-cost applications requires designs that focus on ease of manufacturability and robustness with respect to structural imperfections and nonideal substrates. It also requires the use of inexpensive, earth-abundant metals such as Al for plasmonic properties. In this study, we focus on combining two aspects of plasmonic metasurfaces- visible coloration and Fano resonances- in a morphology amenable to scalable manufacturing. The resulting plasmonic metasurface is a candidate for colorimetric sensing. We examine the potential of this metasurface for strain sensing, where the periodicity of the meta-atoms is modified, and for localized surface plasmon resonance (LSPR) refractive index sensing. This study evaluates the potential of streamlined meta-atom design combined with low-cost metallization for inexpensive sensor readout based on human optical perception.



## **The role of long-range interactions in transport of interacting molecular motors**

**Cade Spaulding**, Hamid Teimouri and Anatoly B. Kolomeisky

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Motor proteins are special enzymes that drive biological transport in living cells by converting chemical energy into mechanical work. Recent experimental evidences suggest that a class of biological motor proteins interact with each other. Stimulated by these observations, we developed a new version of totally asymmetric simple exclusion process with next nearest-neighbor interactions. A theoretical framework based on cluster mean-field approximation, which partially takes correlation into account, is developed to determine the stationary properties of the system. It is found that the nature of the flux-density relation depends on the strength of interactions. Theoretical calculations generally agree with the results from Monte-Carlo simulations, suggesting that our theoretical method correctly describes the main characteristics of the transport of interacting motor proteins with next nearest-neighbor interactions.

## **Spectroscopic Signatures of Plasmon-Induced Charge Transfer in Gold Nanorods**

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Plasmon-induced charge transfer has been studied for the development of plasmonic photodiodes and solar cells. There are two competing mechanisms by which a plasmonic nanoparticle can transfer charge to an adjacent material, indirect transfer after plasmon decay and direct transfer as a mechanism of decay. Using single-particle darkfield scattering and photoluminescence imaging and spectroscopy of gold nanorods on various substrates, we identify linewidth broadening and photoluminescence quantum yield quenching as key spectroscopic signatures that are quantitatively related to plasmon-induced interfacial charge transfer. We find that darkfield scattering linewidth broadening is due to chemical interface damping through direct charge injection via plasmon decay. The photoluminescence quantum yield quenching is indicative of indirect charge transfer following plasmon decay, but prior to charge recombination. Through these two spectroscopic signatures, we identify charge transfer mechanisms at TiO<sub>2</sub> and ITO interfaces and uncover material parameters contributing to plasmon-induced charge transfer efficiency such as Schottky barrier height and resonance energy.

# Undergraduate Student Posters

## **Fabrication, Characterization and Transfer of 2D Materials for THz Spectroscopy**

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2D materials such as MoS<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub>, CrI<sub>3</sub>, hBN, and graphene exhibit exciting and novel physical properties when they are reduced to atomically thin layers, more specifically when they are reduced to monolayers. Many studies have been done to prove their use and efficiency in future electronics. Possible contributions include memory storage, power efficiency, evolution of the transistor, LEDs, photodetectors, and optical modulators, etc. Monolayers can be taken and implemented to become part of a 2D van der Waals heterostructures. Stacking of 2D layered crystals to form van der Waals heterostructures through transfer provides variations in observations which contributes versatility in nanomaterial engineering. This exciting field of research has gained much interest due to the promising discoveries that have been made and the vision of a new generation of electronics resulting from monolayers and their 2D van der Waals heterostructures. In this work we fabricate high quality transition metal dichalcogenide (TDMC) monolayers using the mechanical exfoliation method, with the largest sample being over 60um by 60um in size. The quality of the samples is tested by optical characterization techniques including photoluminescence and second harmonic generation. Monolayers can also be transferred to transparent substrates where the phonon interaction properties a structure may have using THz pump-probe spectroscopy. This work contributes to 2D van der Waals heterostructures and to developing a better understanding of carrier-lattice behavior.

## **Removal of Arsenic from Water Using Fe-nanoparticles impregnated in Fe-Crosslinked Chitosan Beads**

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We studied the removal of arsenate (As(V)) from drinking water by conducting batch and column experiments using Fe-nanoparticles impregnated in Fe-crosslinked chitosan beads. We compared the adsorption of 100 ppb As onto three different Fe-crosslinked chitosan beads, two of which were impregnated with Fe-nanoparticles: {001}-faceted nanoplates (001), {012}-faceted nanocubes (012), and a control bead without nanoparticles (C). We also compared the performance of each material in a solution containing either 25 mM acetate buffer or 0.01 mM NaCl. Batch experiments conducted for 10 days show the three materials tested in both types of solutions can remove As(V). We did not observe significant differences of As removal by using the Fe-nanoparticles facets impregnated on the chitosan beads in the batch experiments. Column experiments using the control beads in the 0.1mM NaCl solution show the removal of As(V) meeting the USEPA maximum contaminant level (10ppb) for 1680 BVs. Breakthrough was not observed after treating 4000 BVs. Our results show that chitosan beads can be used to remove As and that Fe nanoparticles can be a promising strategy to increase the adsorption of As onto chitosan beads in a packed-bed water treatment system. Further work should be conducted to test the feasibility to use Fe-nanoparticles impregnated in chitosan beads for point-of-use- water treatment technologies.

## Thermal Transistor

Andrea Fabila,<sup>1</sup> Dr. Qing Zhu,<sup>1</sup> and Dr. Geoff Wehmeyer<sup>1</sup>

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Electrical transistors are what make all of our computers, phones and other electronics possible and have had a huge impact on the world. We propose a similar device instead, using heat in order to revolutionize energy harvesting and thermal management. Current knowledge and experiments have shown that neodymium and gadolinium can act as magnets. Neodymium which is not a temperature ( $T$ ) dependent magnet and gadolinium which is. At low  $T$  gadolinium has strong magnetization, and at high  $T$  has weak magnetization. A device using these materials would be able to control the flow of heat with a simple design. Three pieces of copper will be used with embedded neodymium. We can label two metals as drain ( $T_d$ ) and source ( $T_s$ ) and the third one gate ( $T_g$ ).  $T_g$  is responsible for the make and break contact between the drain and source. The closing of  $T_g$  at high gadolinium temperatures will allow heat to flow from  $T_d$  to  $T_s$ . Numerical simulations have been used in order to prove this theory, by applying different  $T$  to  $T_d$ ,  $T_s$  and  $T_g$  to export data and graph the success of heat flow between  $T_d$ - $T_s$  at the closing of the gate. The results of this research will lead the theory into prototyping and continue to guide future experimental demonstrations as well.

## Effectiveness of Electrocatalytic Reactors at the MobileNEWT Testbed in Removing Various Contaminants in Water

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In the electrocatalytic process, the *electrochemical reaction* occurs on the catalyst electrode surfaces. The two electrocatalytic reactors available at the MobileNEWT testbed were used during this study to remove contaminants in water. The targeted contaminants included nitrite, nitrate, and PFOA due to being known as toxic organics in water. The two electrocatalytic reactors at MobileNEWT are the *Magneli*, which is equipped with stainless-steel as the cathode and titanium as the anode. While the *ElectroCell* is equipped with boron-doped diamond (BDD) and dimensionally stable anode as cathode and anode respectively. Reactions occur on electrode surfaces in either oxidizing (anode) or reducing (cathode) targeted contaminants in water. Sodium sulfate was used as an electrolyte during this study. The electrocatalytic setup at the MobileNEWT included the reactor, a power supply, a recirculation pump, and a reservoir. During this study, the voltage, amperage, flowrate, pH, and electrolyte solution concentration were varied to maximize targeted contaminant removal. All these runs were for 2-4 hours. A bench-scale study was also performed parallelly using BDD as the electrode. Results show that nitrite could easily be removed (>90%) by the electrocatalytic process, while only a moderate amount of nitrate (29%) and an insufficient amount of PFOA (<5%) could be degraded. Reducing the flow rates or increasing the electrical potential (amp/cm<sup>2</sup>) on electrodes was shown to improve overall removal for some contaminants but less so for others. This research indicates that some pollutants are easier to degrade electrocatalytically. In contrast, others are more difficult to remove, therefore further optimization is necessary.

## **Lithium Deposited Filament Analysis and Oxidation Mitigation with Polyacrylonitrile**

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Current rechargeable lithium batteries, using graphite anodes are near their theoretical energy density limits. With the lowest standard potential (-3.04) and high specific capacity, lithium metal anodes are the ideal successor. However, unstable filament growth during cycling and the highly reactive nature of lithium poses safety and efficiency issues. Study of the filament morphology and growth mechanisms is required to have a better understanding of this complex structures; thus, the formation of Li dendrites can be prevented. There is a need to increase the scale and accuracy of the filament morphology measurements, as well as provide more time to work with the lithium deposited samples in the ambient atmosphere. The Li, when exposed to the atmosphere, produces both Li-oxide and Li-nitride preventing the quality of characterization techniques like SEM imaging. This project utilizes script measurements to analyze the mossy filament structure, also the effects of using a polymer coating to extend the experimental time of the lithium deposited samples are being investigated. Polyacrylonitrile (PAN) at 5% by weight shows a reduction in oxidation time and has a 0.25 $\mu$ m difference in the filament size compared to the control sample. PAN by 1% weight has shown to be useful for scanning electron microscopy (SEM) imaging, and when coated properly, visible, non-oxidized Li still remain after 5 min. Script measurements are promising in being able to produce accurate radius measurements of the Li filaments and only deviate slightly from manual measurements. This is possibly due to the subjective nature in choosing which filaments to take manual measurements of the complex structures.



## **Non-Platinoid Bimetallic Electrocatalysts Overcome Nitrate Reduction Performance of Conventional Platinum Group Electrodes**

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Nitrate is one of the most common pollutant in surface and groundwater, ranked as one of the top ten water violations reported worldwide. Nitrate is linked to several health risks such as blue baby syndrome, cancer, and thyroid problems. Electrocatalytic nitrate conversion has been considered as an attractive alternative due to its environmental friendliness, low cost, and selectivity to transform nitrate to nitrogen gas or ammonia. Bimetallic Electrocatalysts based on copper foam modified with metal nanoparticles, Cu-M (M = metal), hold the promise of enhancing selectivity and kinetics performance. In this study, copper foam was nano-enabled with earth abundant materials (M = Ni, Sn, Cu, and Co) to evaluate synergistic effects of bimetallic centers on nitrate reduction kinetics and selectivity. Electrocatalysts morphology was characterized. Nitrate conversion and selectivity were evaluated at different current densities. Furthermore, electrical energy per order as engineering figure of merit of each material was presented to identify more sustainable nano-modified electrocatalytic systems to nitrate conversion from drinking waters.

## **Analysis of Carbon Nanotube Purification Parameters and Their Effect on Phase Behavior and Aspect Ratio of Carbon Nanotube Solutions**

Dominic Schooley,<sup>1</sup> Michelle Duran-Chaves<sup>2</sup>, Ivan Rosa de Siqueira<sup>2</sup>, and Matteo Pasquali<sup>2</sup>

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Carbon nanotubes (CNTs) have the potential to be large scale manufactured into high-performance materials that find important applications in the structural, energy, aerospace, and biomedical industries, just to name a few. This is due to their highly attractive material properties (mechanical strength, electrical conductivity, and thermal conductivity) combined with light weight and flexibility. To produce CNT macroscopic materials like films and fibers, the purification parameters must be optimized to yield the purest CNTs possible with the aim of obtaining the best performing properties. The purification process includes air oxidation to remove amorphous carbon, HCl wash to remove to remove metallic particles, an overnight H<sub>2</sub>O wash, then a drying sequence. Each trial of purification is subject to polarized optical microscopy and extensional viscosity measurements. The prior used to determine how well dissolved CNTs become in solutions, along with its respective liquid crystalline phase behavior, while the latter is used to determine CNT aspect ratio (CNT length-to-diameter ratio). We tested different purification parameters, such as temperature and time, and assessed their impact on the phase behavior and resulting aspect ratio of CNTs. These intrinsic properties are key to ensure good quality CNT dopes for manufacturing high-performance CNT fibers.

## Carbon Nanotube Fiber Cyclic Tensile Test

Jerardo E. Sanchez,<sup>1</sup> Oliver S. Dewey,<sup>1</sup> Glen C. Irvin<sup>2</sup>, and Matteo Pasquali<sup>3</sup>

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Carbon nanotube fibers (CNTF) can be made from solutions of carbon nanotubes (CNTs) dissolved in chlorosulfonic acid (CSA) using a wet-spinning technique. CNT solutions are extruded through a spinneret and into a coagulation bath for solidification. CNTF produced with this technique have higher tensile strength than metals and many commercially available polymeric and carbon fibers. In order to scale CNTF production to industrial levels, we need to consider the efficiency, cost, and environmental impact. One way to improve these metrics is to use higher concentrations of CNT in the spinning solutions which reduces the amount of acid solvent and non-solvent used per meter of fiber. However, fibers made from lower concentration CNT solutions have higher tensile strengths than those made from higher concentration solutions. To further understand the fiber's microscopic structure as a function of concentration, we performed cyclic tensile tests on fibers made from CNT solutions with concentrations of 1%, 3%, 5%, and 10%. We use these tests to measure the mechanical properties of the CNTF (such as ultimate tensile strength, Young's modulus, and elongation at break) as a function of total strain, strain rate, and number of elongation cycles. Additionally, we can then calculate the energy stored or dissipated in elastic deformations, and the onset of plastic tensile deformations. We find that applying repeated strain cycles improves CNTF Young's modulus and (increases/decreases/leaves the same) the fiber tensile strength. We can then use this information for spinning optimization and design of post-processing techniques such as continuous fiber drawing.

**Title:** Approaching Fast, Multi-Channel Magnetogenetic Cell Activation**Author:** Joseph Asfour<sup>1</sup><sup>1</sup>Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA**Abstract***Introduction*

Genetically-targeted cell activation offers high spatial precision for neural stimulation and cell-based therapies. Magnetic control of cell activity or "magnetogenetics" is a non-invasive method of stimulation which couples magnetic nanoparticle heating in an alternating magnetic field with temperature-sensitive ion channels expressed in select neural circuits. However, two issues currently hinder the widespread adoption of magnetogenetics: 1) temporal latency and 2) multi-channel stimulation. Specifically, the delay between magnet application and *in vivo* behavioral response is currently tens of seconds, and only very few channels can be selectively activated. Seeking to reduce temporal latency, we hypothesize that there exists a species variant of a rate-sensitive thermoreceptor (TRPA1) which is compatible with magnetogenetics in mammals. With an ion channel that responds more strongly to a high rate of temperature change than to an absolute temperature threshold, we could controllably activate cells at temperatures closer to the baseline and hence more quickly. Additionally, seeking to introduce more stimulation channels, we hypothesize that mixing different types of pure nanoparticle populations can generate combined populations with distinct heating properties. Thereby, localizing these distinct populations each to a different neural circuit could enable selective and independent activation of more circuits than currently attainable.

**Electrothermal Membrane Distillation for Minimum or Zero Liquid Discharge**

—Josue Montemayor<sup>1</sup>, Vedant Patel<sup>1</sup>, Naomi Fuentes<sup>2</sup>, Ibrahim Abdallah<sup>2</sup>

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<sup>2</sup>*(NEWT) Department of Civil and Environmental Engineering, Rice University, Houston, TX, USA*

Electrothermal Membrane Distillation (EMD) is a thermally driven process that separates water and salt in hypersaline brine waste toward minimum or zero liquid discharge. EMD is based on using thermal elements over a hydrophobic membrane. The thermal coating element of the membrane is connected to a power supply. When a certain electric voltage is applied, the thermal heating element generates Joule heat that is conducted to the adjacent feed water. The heated feedwater is evaporated at the interface and the vapor transferred to the permeate side. One of the major challenges towards the applicability of EMD is chemical corrosion of the thermal elements. Batch experiments were conducted on small scale for evaluating different anticorrosion nanocoating materials, including activated carbon and polymer coatings (PTFE, Nycote-99 single, silicone, Flex Seal) at different power densities using 100,000 ppm NaCl synthetic brine. The results revealed that Nycote-99 is the most viable coating to protect thermal elements (316 stainless steel). In addition, a tubular EMD reactor was designed, developed, and tested using hypersaline simulated NaCl solutions (100,000 ppm NaCl). The performance of the EMD reactor was tested under different operating conditions. Going forward, other levels of coating will be tested to compare to Nycote-99 as an alternative. The Tubular EMD reactor proved to be effective and will continue to be designed and improved on.

## Promoting Plasmid Stability and Bioremediation Through the Spread of Engineered *bphC* Dioxygenase Activity

Katie Impelman<sup>1</sup>, Tessa Crosby<sup>2</sup>, and Lauren Stadler<sup>2</sup>, PhD

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Inserting *bphC*, a dioxygenase enzyme, into microbes via conjugation enables them to degrade 2,3-dihydroxybiphenyl, a model polycyclic aromatic hydrocarbon (PAH). There is little research on how long the *bphC* gene persists in a population of recipient bacteria over time, which is necessary for employing bioremediation initiatives within relevant environments. The objective of this project is to determine to what extent selective pressures, including antibiotic resistance and the presence of substrate in media, affect the stability of two disparate plasmid constructs with the *bphC* gene across generations. We performed a ten-day serial growth experiment that compared the effectiveness of *E. coli* DH10B transconjugants consisting of two *bphC* engineered plasmid backbones: TP114 and RSF1010. Each day, we collected OD600 measurements to measure cell growth, sequenced the plasmid to confirm presence of *bphC* gene, plated on antibiotic selective plates to record the number of colony forming units (CFUs) with plasmid, and performed a functional assay to monitor how rapidly the recipient cells degraded substrate over time. Our results revealed that selective pressure does impose a fitness burden on the bacteria. In media conditions with antibiotic, following an acclimation period, the cells with the smaller plasmid, RSF1010::*bphC*, were able to proliferate unlike the cells with the larger plasmid, TP114::*bphC*. We also found that the presence of the substrate in media caused the cells to grow significantly slower, leading us to believe that the 2,3-dihydroxybiphenyl byproduct is toxic. Since growing one cell-type in laboratory media does not replicate complex community interactions, the applications of our results are limited. However, our results help future researchers understand the pressures to which plasmids engineered with *bphC* are susceptible.

## **Controlling the Expression of Adhesins**

Keyla V. Ramirez,<sup>1</sup> Nicolas E. Grandel,<sup>2</sup> and Matthew R. Bennett<sup>3</sup>

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Microbial communities have the capability of advancing environmental restoration efforts through bioremediation. Microbial consortia improve the efficiency of a system but are difficult to control. Focusing on spatial control can make these communities more manageable. Currently, adhesins are being used to advance spatial control. Adhesins are pairs of mutually-adhesive surface-displayed proteins that bind to the cell wall of bacteria that have specific receptors. The shape of cell aggregates can be altered by controlling the expression of adhesins. This can help breakdown waste through adhesins latching onto microplastics better. This research project will try to control the expression of adhesins to make microbial aggregates of a pre-defined size and shape. By tightly regulating the average adhesin number in two different strains, we hope to create “bullseye”-like shapes composed of a single cell surrounded by a monolayer of its conjugate strain.

## Selective Electrosorption for Scaling and Fouling Control

Victory Amos-Nwankwo<sup>1</sup>, Sharifa Akbary<sup>1</sup>, Mark Hanna<sup>1</sup>, Naomi Fuentes<sup>2</sup>, Ibrahim Abdallah<sup>2</sup>

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Selective Electrosorption (SES) is an electrochemical process for treating industrial wastewater using selective porous electrodes. SES is based on applying an electrical potential difference over the electrodes, which are made of porous selective nanomaterials designed to remove specific scaling ions from the wastewater. The SES reactor consists of different components, including 12 ion-selective electrodes with a total electrode area of 0.17 m<sup>2</sup>, and a surface area of 2,040 m<sup>2</sup>/g. Graphite sheets were used as current collectors, cation exchange membranes, anion exchange membranes, and 1-mm-thick woven nonconductive mesh spacer (61% porosity) for creating flow channels. Many parameters affecting the performance of the selective electrosorption technology, including the feed flow rate, applied potential difference, operating temperature, and initial feed concentration. In this work, the impact of temperature on the reactor's adsorption capability to remove scaling ions has been executed using two levels of operating temperature (25° C and 45° C) at 1.2 volts. Additionally, two levels of applied potentials (1.2 V and 0.6 V) have been examined for evaluating the performance of the SES toward scaling mitigation using different scaling ions and concentrations (Na<sub>2</sub>SO<sub>4</sub>, NaCl, CaCl<sub>2</sub>). The results showed that higher temperature (45° C) corresponded to higher effluent conductivity and lower salt adsorption capacity. This could be attributed to the exothermic behavior of the SES.



## Development of metal dichalcogenide coated acupuncture needles for NO biosensing

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NO is an important signaling molecule involved in physiological functions, difficult to detect directly due to its high reactivity. We aimed to develop a highly sensitive NO biosensor by coating acupuncture needles with MoS<sub>2</sub> or FeS for the purpose of rapid, minimally invasive health diagnoses. The biosensor is composed of a stainless-steel needle with an FeS coated tip formed through chemical vapor deposition (CVD). The MoS<sub>2</sub> coating was formed using hydrothermal synthesis. The biosensing electrode was prepared by applying a UV-curable epoxy to the needle base, and cyclic voltammetry tests confirmed its sensing capabilities through detected redox reactions of NO in the solution. The MoS<sub>2</sub> and FeS coating compositions were characterized through scanning electron microscopy (SEM) and x-ray photoelectron spectroscopy (XPS). *In vitro* testing will be conducted in the future to determine clinical feasibility.

## Riya Narayan Abstract for Graphene-Based Supercapacitor Electrodes

Graphene shows very high prospects in the energy storage systems due to its high surface area ( $2630\text{m}^2/\text{g}$ ) and excellent electrical conductivity, especially, in electrochemical double layer supercapacitors. However, graphene poses a lot of problems such as restacking of its layers and improper adhesion of the coatings on the current collectors. One way to overcome this issue is to utilize the correct binder for proper adhesion and utilizing the surface area of graphene in supercapacitor electrodes. In this study, we analyze the effect of different commercially available binders on graphene electrodes using cyclic voltammetry and impedance spectroscopy.

## **Visualizing paramagnetic colloidal dimer interactions under rotational magnetic field**

Lisa Biswal,<sup>1</sup> Kedar Joshi<sup>1</sup>, and Ros'Lynn Charles<sup>1</sup>

<sup>1</sup>*R-STEM Nano REU: Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas, U.S.A*

Paramagnetic colloids are one of the types of active matter. Paramagnetic colloids acquire induced magnetic dipole as we apply external magnetic field. Induced dipole allows particles to interact with one another. By controlling the magnetic field, we can fabricate different microstructures and create different dynamics. Rotational magnetic field (RMF) is well studied topic which results in attractive potential between particles. It is known that under high frequency rotational magnetic field (HERMF) superpara magnetic colloids undergo a phase transition from uniformly distributed to cluster phase. It was assumed in the research community that magnetic dipole is instantaneously developed in super paramagnetic colloids. This is good assumption for constant field or slowly time varying field, but fails at faster time varying fields. If you have fast changing magnetic field there is a delay between field direction and induced dipole inside super magnetic colloids. This delay is refereed as relaxation time, which causes particle clusters to rotate under HERMF. We have developed a new back-and-forth RMF to cancel out the rotation inside clusters. However, on a larger scale this back-and-forth field creates an anisotropic structure, which were not observed in the traditional HERMF. We have studied particle interactions by observing a pair of particles under both rotational and back and forth field. Interaction potential between a particle pair as a functions of fields frequency gives interesting insight about the relaxation time.

**Electrothermal Membrane Distillation for Minimum or Zero Liquid Discharge**

—Josue Montemayor<sup>1</sup>, Vedant Patel<sup>1</sup>, Naomi Fuentes<sup>2</sup>, Ibrahim Abdallah<sup>2</sup>

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Selective Electrosorption (SES) is an electrochemical process for treating industrial wastewater using selective porous electrodes. SES is based on applying an electrical potential difference over the electrodes, which are made of porous selective nanomaterials designed to remove specific scaling ions from the wastewater. The SES reactor consists of different components, including 12 ion-selective electrodes with a total electrode area of 0.17 m<sup>2</sup>, and a surface area of 2,040 m<sup>2</sup>/g. Graphite sheets were used as current collectors, cation exchange membranes, anion exchange membranes, and 1-mm-thick woven nonconductive mesh spacer (61% porosity) for creating flow channels. Many parameters affecting the performance of the selective electrosorption technology, including the feed flow rate, applied potential difference, operating temperature, and initial feed concentration. In this work, the impact of temperature on the reactor's adsorption capability to remove scaling ions has been executed using two levels of operating temperature (25° C and 45° C) at 1.2 volts. Additionally, two levels of applied potentials (1.2 V and 0.6 V) have been examined for evaluating the performance of the SES toward scaling mitigation using different scaling ions and concentrations (Na<sub>2</sub>SO<sub>4</sub>, NaCl, CaCl<sub>2</sub>). The results showed that higher temperature (45° C) corresponded to higher effluent conductivity and lower salt adsorption capacity. This could be attributed to the exothermic behavior of the SES.

## **Characterizing Sulfonated Pentablock Terpolymer NEXAR as Pervaporation Membrane for Treatment of Inland Desalination Concentrates**

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Reverse osmosis (RO) is the current leading water desalination technology worldwide. One of the critical challenges RO faces is the management of inland desalination concentrates. Alternative technologies, such as pervaporation (PV), are being studied as a solution for this problem. In this project, freestanding dense pervaporation membranes made from a sulfonated pentablock terpolymer with the trade name of NEXAR™ were characterized. The NEXAR™ polymer was available in four charge densities: MD9100, MD9150, MD9200, and MD9260, with MD9100 being the lowest and MD9260 the highest. NEXAR membranes were individually casted using a film casting knife. Commercially available membrane distillation (MD) membranes and DeltaMem membranes were tested to compare performance results of NEXAR membranes. Salt rejection and flux performance of each charge density were measured using a Sterlitech HP4750 high pressure cell. Surface charge was measured using a zeta potential meter ZetaCAD. The average salt rejection for MD9100 was 12.5%, for MD9150 was 7.5%, for MD9200 was 6.3%, and for MD9260 was 0%. It was found that salt rejection decreases as charge density increases, while flux increases as the charge density increased. Further research is required to continue fully characterizing the NEXAR polymer.