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SCI Summer Research Colloquium
August 4, 2023

2023 Smalley-Curl Summer Research Colloquium

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NSF Nanosystems Engineering Research Center for
Nanotechnology Enabled Water Treatment Systems (NEWT)

Schedule

8:00 am Breakfast and registration (Martel Hall)
8:55 am Introductory remarks (McMurtry Auditorium)

Oral session A (McMurtry Auditorium)

Session Chair: Elijah Kritzell

9:00 am **Aleida Machorro Ortiz** "Solar Thermal Resonant Energy Exchange Desalination for Off-grid Brine Concentration"
9:12 am **Wei Meng** "Next-generation 2D Optical Strain Mapping with Strain-Sensing Smart Skin (S4)"
9:24 am **Ziyang Wang** "Measuring complex refractive index through deep-learning-enabled optical reflectometry"
9:36 am **Jacques Doumani** "Ordered Carbon Nanotube Assemblies with Synthetic Chirality"
9:48 am **Rui Xu** "Phonon Polaritonics in Broad Terahertz Frequency Range with Quantum Paraelectric $SrTiO_3$"

Keynote

10:00 am – 10:30 am **Hanyu Zhu** "Chiral phonons, a new route for quantum control"

Oral Session B (McMurtry Auditorium)

Session Chair: Kiran Muralidhar Kulkarni

11:00 am **Wenjing Wu** "Chip-scale Manufacturing of Highly Uniform Single Crystal 2D Materials"
11:12 am **Tymofii Pieshkov** "Phase transitions in thin films of WSe2 induced by the in situ heating"
11:24 am **Ulises Felix Rendon** "Observation of single T centers in silicon nanophotonic structures"
11:36 am **Elijah Kritzell** "Simulation of the Dicke Model in the Ultrastrong Coupling Regime Using Paramagnetic Spins"
11:48 am **Haad Rathore** "Large-scale, Longitudinal Neural Recordings Reveal Spatially Graded, Cell-Type Specific Plasticity Following Small-Scale Ischemic Strokes"

12:00 pm – 1:00 pm **Lunch** (Martel Hall)

1:00 pm – 3:00 pm **Poster Session** (Martel Hall)

Oral Session C (McMurtry Auditorium)

Session Chair: Will Smith

3:00 pm **Chuqiao Shi** "Four-dimensional Scanning Transmission Electron Microscopy (4D-STEM) on 2D Material and Nano Particles"

3:12 pm **Tong Lin** "Sub-wavelength, phase-sensitive microscopy of third-order nonlinearity in terahertz frequencies"

3:24 pm **Yiyi Yang** "A Novel Computational Approach for Predicting Colors in Van der Waals Layered 2D Materials: Implications for Material Characterization and Device Applications"

3:36 pm **Dongjoo Lee** "Novel Synthetic Approach to Degradable Bottlebrush Polymers with Tailored Side-chains"

3:48 pm **Yigao Yuan** "Photocatalytic steam methane reforming using a plasmonic Cu-Rh antenna-reactor photocatalyst"

Oral Session D (McMurtry Auditorium)

Session Chair: Adam Johnston

4:30 pm **Kiheon Hong** "Nickel Enhances InPd-Catalyzed Nitrate Reduction Activity and N2 Selectivity"

4:42 pm **Sohail Dasgupta** "Finite Temperature Quantum Matter with Rydberg or Molecule Synthetic Dimension"

4:54 pm **Emilie Novak** "Towards Sample-to-Answer HPV 16 and HPV 18 mRNA Detection for Assessing Cervical Cancer Risk"

5:06 pm **Yuxiang Gao** "Anomalous Hall effect in the antiferromagnetic Weyl semimetal SmAlSi"

5:18 pm **Yichen Zhang** "Kramers nodal lines in SmAlSi and other ideal candidates, (Pb/In)TaX_2 (X=S or Se)"

5:30 pm – 6:30 pm **Award Ceremony and Dinner Cocktail** (Martel Hall)

Keynote

Chiral phonons, a new route for quantum control

Hanyu Zhu

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Symmetry is an important concept in condensed matter. The term “chiral” has been applied in many different fields in physics and chemistry to describe the lack of certain symmetry, which leads to fascinating properties from selective interaction and unidirectional transport. The symmetry of non-chiral materials may be broken by the atomic motion of coherently excited “chiral phonons”. Instead of oscillating back and forth around their equilibrium positions, the atoms rotate and maintain a non-zero perturbation at all times to the electrons. Chiral phonons with quantized angular momentum are simply guaranteed by multifold rotational symmetry, and thus are rather common in materials and have been predicted to cause unexpected magnetic, topological, and transport phenomena. In this talk, I will first briefly introduce the history and recent progress of chiral phonon research. I will then introduce a possible classification of chiral phonons, which we tentatively named “Lugano test”, that connects various types of chirality with possible quantum control of functionalities. Finally, I will give the example of controlling spins in magnetic materials with chiral phonons that potentially lead to a new paradigm of dynamic structural-property relationship in quantum materials.

Oral Presentations

OA1 – Solar Thermal Resonant Energy Exchange Desalination for Off-grid Brine Concentration

Aleida Machorro-Ortiz,[1,2] Pratiksha D. Dongare,[1] William Schmid,[1] Alessandro Alabastri,[1] and Naomi J. Halas[1]

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[2]*Applied Physics Graduate Program, Rice University, Houston, Texas, USA*

More than half of the world's population lives in regions with water scarcity, accentuated by overpopulation, climate change, and industrialization. To guarantee freshwater access for current and future generations, sustainable and effective solutions are urgent. Given the abundance of saline water reserves on Earth, reverse osmosis-driven desalination is popularly implemented worldwide, with more than 18,000 desalination plants generating fresh water. With around a 50% water recovery rate, these plants generate 50% brine waste, which gets discharged to nearby water bodies, transported to saltwater disposal wells, or evaporated with large area evaporation ponds. Membrane-based solutions treating high salinity brine waste suffer from scaling, fouling, and membrane maintenance, whereas thermal phase change-based solutions are inherently inefficient due to the required phase change enthalpy.

This work develops a solar thermal resonant energy exchange desalination (STREED) system that efficiently uses incident solar energy for brine concentration through resonant energy transfer. STREED is membrane-free, modular, and dynamically tunable with incident sunlight intensity to optimize system performance throughout the day. The core principle of resonant energy transfer allows storing incident sunlight energy in STREED through the efficient recovery of phase change enthalpy, enabling operation even beyond sunset. This system can achieve specific water production of >3 L/kWh, making it attractive for real-life applications. STREED can significantly boost the water recovery of existing desalination systems and reduce the generated brine waste, enabling sustainable and environmentally conscious desalination practices to secure our planet's water future.

OA2 – Next-generation 2D Optical Strain Mapping with Strain-Sensing Smart Skin (S^4)

Wei Meng,[1] Ashish Pal[1], Sergei M. Bachilo[2], R. Bruce Weisman[2,4] and Satish Nagarajaiah[1,3,4]

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Strain-sensing smart skin (S^4) is a novel solution to the widespread industrial need for non-contact strain measurement. We have developed single-walled carbon nanotubes as microscopic strain sensors. Nanotubes are dilutely dispersed in a polymer coating that is applied to the structure's surface in a thin protective film that also senses strain. In this method, strain at any position on the surface can be quickly measured by shining a laser beam onto the film, collecting the nanotube fluorescence, and analyzing the spectrum. To map strain over the whole surface, we can either scan the S^4 measurement device and compile the set of readings or use a recently developed hyperspectral imaging device. By applying S^4 on critical structures, one can easily measure accumulated strain, identify damage locations, and evaluate structural health. Noncontact strain maps measured with the S^4 films were directly compared to those from the established digital image correlation (DIC) method on plastic, concrete, and aluminum test specimens, including one with subsurface damage[1]. Strain features were more clearly revealed with S^4 than with DIC. Finite element method (FEM) simulations also showed closer agreement with S^4 than with DIC results. These findings highlight the potential of S^4 strain measurement technology as a promising alternative or complement to existing technologies, especially when accumulated strains must be detected in structures that are not under constant observation.

[1] Meng, Wei, Ashish Pal, Sergei M. Bachilo, R. Bruce Weisman, and Satish Nagarajaiah. "Next-generation 2D optical strain mapping with strain-sensing smart skin compared to digital image correlation." *Scientific reports* 12, no. 1 (2022): 11226.

OA3 – Measuring complex refractive index through deep-learning-enabled optical reflectometry

Ziyang Wang,[1] Yuxuan Cosmi Lin,[2] Kunyan Zhang,[1,3] Wenjing Wu,[1,4] and Shengxi Huang[1]

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Optical spectroscopy is indispensable for research and development in nanoscience and nanotechnology, microelectronics, energy, and advanced manufacturing. Advanced optical spectroscopy tools often require both specifically designed high-end instrumentation and intricate data analysis techniques. Beyond the common analytical tools, deep learning methods are well suited for interpreting high-dimensional and complicated spectroscopy data. They offer great opportunities to extract subtle and deep information about optical properties of materials with simpler optical setups, which would otherwise require sophisticated instrumentation. In this work, we propose a computational approach based on a conventional tabletop optical microscope and a deep learning model called ReflectoNet. Without any prior knowledge about the multilayer substrates, ReflectoNet can predict the complex refractive indices of thin films on top of these nontrivial substrates from experimentally measured optical reflectance spectra with high accuracies. This task was not feasible previously with traditional reflectometry or ellipsometry methods. Fundamental physical principles, such as the Kramers-Kronig relations, are spontaneously learned by the model without any further training. This approach enables in-operando optical characterization of functional materials within complex photonic structures or optoelectronic devices.

OA4 – Ordered Carbon Nanotube Assemblies with Synthetic Chirality

Jacques Doumani[1,2,3] Minhan Lou,[3] Oliver Dewey,[4,5] Nina Hong,[6] Jichao Fan,[3] Andrey Baydin,[1,7] Matteo Pasquali,[4,5,7,8,9] Yohei Yomogida,[10] Kazuhiro Yanagi,[10] Riichiro Saito,[11] Junichiro Kono,[1,4,7,9,12] and Weilu Gao[3]

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[12]*Department Physics and Astronomy, Rice Univ., Houston, TX, USA*

Controlling the dissymmetric interaction of circularly polarized light with solid-state materials is crucial for developing chiral photonic systems. While the molecular-level chirality of chiral carbon nanotubes (CNTs) has shown circular dichroism signals in enantiomer-enriched CNT suspensions, the rotatory power is too small for practical applications. Achieving macroscopic assemblies of ordered CNTs with engineered chiroptical properties remains a challenge.

In this study, we demonstrate tunable, giant, and structure-induced deep-ultraviolet circular dichroism in wafer-scale films of ordered racemic CNTs using two approaches. The first approach involves mechanical-rotation-assisted vacuum filtration, while the second approach focuses on 3D chiral stacking of aligned CNTs. By adjusting the rotation forces and twist angles in the respective approaches, we can engineer the chirality, including the strength and sign of circular dichroism. Our experimental data, confirmed by transfer-matrix calculations and full-wave electromagnetic numerical simulations, showcases a record high ellipticity of 40 mdeg/nm. Our theoretical simulations predict that a film of twist-stacked CNTs with an optimized thickness will exhibit an even higher ellipticity of up to 150 mdeg/nm.

These advancements in tunable deep-ultraviolet circular dichroism provide a promising platform for various applications. The chiral assembly of quantum wires using these techniques holds significant potential for secured communication, deep-sea imaging, and chiral quantum emission. These methods offer simplicity, reproducibility, and scalability, opening up new avenues for the development of large-scale chiral photonic systems.

OA5 – Phonon Polaritonics in Broad Terahertz Frequency Range with Quantum Paraelectric $SrTiO_3$

Rui Xu,[1] Tong Lin,[1] Jiaming Luo, [1,2] Xiaotong Chen,[1] Elizabeth Blackert, [1] Alyssa Moon, [3] Khalil JeBailey[1] and Hanyu Zhu[1]

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Photonics in the frequency range of 5 to 15 terahertz (THz) potentially open a new realm of quantum materials manipulations and biosensing. This range, sometimes called "the new terahertz gap", is traditionally difficult to access due to prevalent phonon absorption bands in solids. Low-loss phonon-polariton materials may realize sub-wavelength, on-chip photonic devices, but typically operate in mid-infrared frequencies with narrow bandwidths and are difficult to manufacture in large scale. Here for the first time, quantum paraelectric SrTiO3 enables broadband surface phonon-polaritonic devices in 7–13 THz. As proof of concept, polarization-independent field concentrators are designed and fabricated to locally enhance intense, multicycle THz pulses by a factor of 6 and increase the spectral intensity by over 90 times. The time-resolved electric field inside the concentrators are experimentally measured by THz-field induced second harmonic generation. Illuminated by a table-top light source, the average field reaches 0.5 GV/m over a large volume resolvable by far-field optics. Our results potentially enable scalable THz photonics with high breakdown fields made of various commercially available phonon-polariton crystals for studying driven phases in quantum materials and nonlinear molecular spectroscopy.

OB1 – Chip-Scale Manufacturing of Highly Uniform Single Crystal 2D Monolayers

Wenjing Wu,[1,2] Junichiro Kono,[1,3,4,5] and Shengxi Huang[1,4]

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Research in two-dimensional (2D) materials has surged due to their novel physical properties and potential applications in optoelectronics. 2D materials, with their unique potential to revolutionize electronics and photonics, have captured the interest of scientists across disciplines. Recent advances have seen significant strides in growing 2D monolayers over large areas, a development crucial for transitioning this research from the lab to industry. However, a major roadblock remains: it has not been possible to achieve high-quality single crystallinity and a large lateral size simultaneously in monolayer production for industrial applications. Here, we present a facile method that can yield large-area single-crystal 2D monolayers, displaying remarkable uniformity and crack-free merits. This innovative process takes advantage of gold tape and a wafer bonder, which are compatible with standard semiconductor fabrication techniques, augments existing knowledge, and moves us a step closer to realizing the widespread industrial applications of 2D monolayers.

OB2 – Phase transitions in thin films of WSe_2 induced by the in situ heating

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Materials scientists have long been working on engineering 2D materials into the next generation of nanoelectronic devices. Among all 2D materials, transition metal dichalcogenides (TMDs), like WSe_2, can exist simultaneously in two phases with 2H having semiconducting and 1T having metallic properties. This creates opportunities for using WSe_2 as both source/drain electrodes as well as a semiconductor in between them. Thus, understanding and engineering of phase transitions would provide a key to unlocking this potential as well as opening up new possibilities of electronic, magnetic, or catalytic properties present in 2D TMDs. Here, we present the steps undertaken and future plans to grow, analyze and induce the phase transition of WSe_2 flakes. The growth of WSe_2 was done in chemical vapor deposition at 750°C on silica wafers after which, the samples were transferred to heating chips for transition electron microscopy (TEM) analysis and *in situ* heating to induce the phase changes. A protective layer of graphene was deposited on top of WSe_2 flakes to make them more resilient to high energy electrons and heating during the experiment to mitigate the damage. The phase transitions between the 1T and 2H were previously reported, but to the best of our knowledge, no *in situ* TEM experiments have demonstrated the transition. We believe that our research will expedite the development of devices with 2D heterostructures via phase engineering.

OB3 – Observation of single T centers in silicon nanophotonic structures

Ulises Felix-Rendon,[1,2] Adam Johnston,[1,2] Yu En Wong,[1,2] and Songtao Chen[1,3]

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In recent years, optically interfaced solid-state spins have attracted increasing attention as promising candidates for the development of quantum networks. This approach allows the creation of hybrid platforms, enabling high-fidelity local manipulation, storage and readout of qubits using electronic and nuclear spins, and outcoupling via spin−photon interfaces for remote spin entanglement generation. One of the novel optically active defect spins is the T center in silicon, which is equipped with advantageous properties for quantum networking applications, including narrow optical transitions in the telecommunication O-band and long-lived electronic and nuclear spins. Benefiting from the mature silicon platform, the T centers can be integrated with photonic devices for better collection efficiency and enhanced light-matter interactions. Early demonstration of single T centers relied on confocal-type measurements, which have a limited photon collection efficiency due to the silicon totally internal reflection. In this work, we observe single T centers in silicon nanophotonic structures using direct fiber coupling. We generate T centers via ion implantation in the device layer of a silicon-on-insulator wafer, where nanophotonic circuits consisting of photonic crystal cavities, linearly tapered waveguides, and grating couplers are fabricated. We perform time-resolved photoluminescence excitation spectroscopy to characterize single T centers and show evidence of their single photon emission. This work represents an important step towards utilizing single T centers in silicon nanophotonic structures for quantum networking applications.

OB4 – Simulation of the Dicke Model in the Ultrastrong Coupling Regime Using Paramagnetic Spins

T. Elijah Kritzell,[1,2] Junzhe Bao,[3] Jacques Doumani, [1,2] Jae Joon lee, [3] Hongjing Xu, [3] Fuyang Tay, [1,2] Hiroyuki Nojiri, [4] Motoaki Bamba, [5,6] Andrey Baydin, [1,7] and Junichiro Kono[1,3,7,8]

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The Dicke model in quantum optics describes the cooperative interaction of an ensemble of two-level atoms with a single mode of light. Theoretical analysis of such hybridized systems offers a number of exciting avenues for new, exotic physics. Over the last decade, phenomena unique to the ultrastrong coupling (USC) regime have been revealed in many light–matter hybrid systems, including large quantum-vacuum-induced effects in condensed matter. However, the matter side of these coupled systems can be usually approximated as a bosonic excitation, making the problem essentially equivalent to that of two interacting simple harmonic oscillators, describable by the Hopfield Hamiltonian. Hence, little is known about spin-boson interactions, whose coupling strength should depend on the population difference between the levels of the system. In addition, the USC of magnetic resonances with cavity photons remains largely unexplored. Here, we study the USC of an ensemble of paramagnetic spins with Fabry–Pérot (FP) cavity photons in $Gd_3Ga_5O_{12}$ (GGG), a paramagnetic insulator, in a magnetic field. By polishing the sample to optimized thicknesses, we formed a cavity structure from the crystal surfaces. GGG contains unpaired electrons, which, in the presence of an external magnetic field, generate an electron paramagnetic resonance (EPR) signal. We perform terahertz magneto-spectroscopy experiments which reveal EPR-polaritons in the USC regime and observe that the coupling strength depends on both temperature and applied magnetic field. These results show that an ensemble of paramagnetic spins coupled with a single cavity mode produces the physical situation described by the original Dicke model, which promises future realizations predicted phenomena such as the superradiant phase transition.

OB5 – Large-scale, Longitudinal Neural Recordings Reveal Spatially Graded, Cell-Type Specific Plasticity Following Small-Scale Ischemic Strokes

Haad Rathore,[1,4] Rongkang Yin,[2,4] Jiaoo Zhang,[2,4] Yifu Jin,[2,4] Fei He,[2] Brian Noble,[1,4] Yingchu Sun[2,4], Pavlo Zolotavin,[2] Chong Xie[1,2,3,4] and Lan Luan[1,2,3,4]

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The brain possesses a remarkable ability to undergo spontaneous self-repair in response to injury such as an ischemic stroke. This dynamic restorative process involves a diverse array of mechanisms that are time and location dependent, defining a distinct therapeutic window, wherein the cortex demonstrates heightened levels of neuroplasticity. Previous studies using 2-photon imaging techniques have shown evidence of structural plasticity but no significant functional remapping at a cellular level following an ischemic stroke. In this study, we use a digital micro-mirror device to create a precise photothrombotic micro-lesion with fine location control. To chronically record neuroactivity from hundreds of neurons, we deployed large-scale, spatially distributed electrophysiology using the ultraflexible neural-thread electrodes. We stimulated the whisker corresponding to the stroked barrel and simultaneously recorded from the peri-infarct tissue, farther-away tissue, and the secondary somatosensory cortex. Classifying cells based on their electrophysiological signatures and tracking the changes in neuronal populations and their firing dynamics for six weeks revealed cell-type specific alterations in functional responses that are highly sensitive to the distance from the infarct-core. Specifically, we observed that one week after the occurrence of a stroke, heightened inhibitory cell population within a limited range of a few hundred micrometers surrounding the core while in the distant cortical tissue as well as the secondary somatosensory cortex, the populational level excitation-inhibition balance remained intact. Finally, we also detected a significant increase in the firing rate of excitatory neurons in the distant regions from the stroke site, indicating first evidence for spatially dependent functional remapping.

OC1 - Four-dimensional Scanning Transmission Electron Microscopy (4D-STEM) on 2D Material and Nano Particles

Chuqiao Shi,[1] Yimo Han[1]

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Scanning transmission electron microscopy (STEM) is a highly effective method of characterization that finds wide application in imaging, diffraction, and spectroscopy. Recent advances in pixelated and fast direct electron detectors allow for the collection of full momentum data from scattered electrons at each scanning position. Combining two scanning dimensions (x, y) in real space and two momentum dimensions (kx, ky), a four-dimensional data can be acquired in the electron microscope, which is referred to as 4D-STEM. Compared with conventional STEM images with one-pixel intensity, 4D-STEM are comprised of a moment-resolved diffraction pattern per scanning point, which provide extremely rich lattice information of materials. Here I will introduce our work of applying 4D-STEM to study different material systems, including revealing the in-plane lattice distortion and out-of-plane stacking information in 2D vdw ferroelectric SnSe, understanding the strain and strain releasing mechanism in core-shell nanoparticles and identify the strain inhomogeneity in the pentatwinned nanoparticles.

OC2 – Sub-wavelength, phase-sensitive microscopy of third-order nonlinearity in terahertz frequencies

Tong Lin,[1] Rui Xu[1], Xiaotong Chen[1], Yuxuan Guan[1], Mingxing Yao[1], Junhao Zhang[1], Xinwei Li[2], and Hanyu Zhu[1]

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[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*

The third-order nonlinear susceptibility $\chi^{(3)}$ occurs universally in materials and can provide label-free fingerprint of materials' electronic, vibrational, and structural information. One quantitative spectroscopic method to access low-energy resonances of $\chi^{(3)}$ is the terahertz electric field induced second harmonic generation (TEFISH), which is particularly suitable for centrosymmetric materials without second-order processes. However, using TEFISH to measure the $\chi^{(3)}$ spectra requires light sources with high spectral intensity, which is challenging for the "new terahertz gap" frequencies between 5 – 15 THz that, not by coincidence, are the fingerprint phonon bands for many materials. Here for the first time, we report phase-sensitive heterodyne TEFISH microscopy offering simultaneous temporal, spectral, and spatial resolution, incorporating intense and frequency-tunable narrowband terahertz source by chirped pulse difference frequency generation in the frequency range of 4 to 18 THz. We demonstrated time-resolved hyperspectral TEFISH microscopy in polymer thin films (SU-8), 2D crystalline semiconductors (MoS_2), and sub-wavelength photonic resonators. By interfering the nonlinear emission with a local oscillator field, we quantitatively retrieved the frequency, amplitude, and relative phase of the $\chi^{(3)}$ spectra. TEFISH microscopy allows time-resolved imaging of vibrational and photonic resonances with sub-wavelength resolution and higher sensitivity compared to linear Fourier transform infrared spectroscopy, as well as versatility for samples in different environments by avoiding near-field probes.

OC3 – A Novel Computational Approach for Predicting Colors in Van der Waals Layered 2D Materials: Implications for Material Characterization and Device Applications

Yiyi Yang,[1]Qin-Kun Li,[1] and Boris I. Yakobson[1]

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

Color, a fundamental property discernible by the human eye, offers profound implications in material science. However, predicting the colors of van der Waals layered 2D materials, renowned for their excellent performance in electronic and optoelectronic devices, remains challenging due to complex atomic structures and varying synthesis techniques. This study employs first-principles calculations and the transfer matrix method to reveal the colors of weakly-bonded layered 2D materials, including the transition-metal dichalcogenide family, graphene, and CrX3 (X=Cl, Br, I). Our results demonstrate a correlation between color and material thickness, confirmed by comparing calculated colors with experimental reports. Single-layer MoS2 appears black, while the 50-layer MoS2 exhibits a unique creamy white color, signifying a color additive property within layered 2D materials. WSe2 showed a similar color pattern, strengthening the reliability of our findings. These results provide a foundation for future investigations on the influence of defects and stacking order on color presentation. By predicting desired colors through fine-tuned material combinations, this work contributes a valuable approach for experimental synthesis and the design of color-oriented devices, catering to applications in diverse fields such as visual aids for color deficiency and devices for animal use. Future steps will explore these applications further and expand our understanding of the optical behavior of layered materials, ushering in new possibilities for this versatile class of materials.

OC4 – Novel Synthetic Approach to Degradable Bottlebrush Polymers with Tailored Side-chains

Dongjoo Lee,[1] Hanqing Wang,[1] and Rafael Verduzco[1,2]

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Bottlebrush polymers have a variety of potentially useful properties including a high entanglement molecular weight, low Young's modulus, and rapid kinetics for self-assembly. However, the translation of bottlebrushes to real-world applications remains limited due to challenging synthetic pathways that rely on expensive reagents and complex, multi-step polymerizations. Additionally, there is a need to develop bottlebrush polymers that can be degraded or recycled. The annual production of polymers is approaching 500 Mt, and the majority of these polymers cannot be easily or economically recycled. Herein, we develop a new synthetic method that enables an inexpensive, versatile, and simple approach to synthesize degradable bottlebrush polymers under mild reaction conditions by using α-lipoic acid (LA) as a bottlebrush backbone. LA is an inexpensive, naturally occurring, and biocompatible small molecule. Due to reversibility of the disulfide bond in LA, resulting bottlebrush polymers could be depolymerized to macromonomers, which could be recycled to produce new bottlebrush polymers. This work enables the inexpensive and large-scale preparation of degradable bottlebrush polymers with variety of side-chain chemistries and will allow us and others to greatly advance the development of bottlebrush polymers.

OC5 – Photocatalytic steam methane reforming using a plasmonic Cu-Rh antenna-reactor photocatalyst

Yigao Yuan[1], Jingyi Zhou[2], Aaron Bayles[1], Hossein Robatjazi[1,3], Peter Nordlander[4,5], Naomi J. Halas[1,4,5]

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Industrial steam methane reforming (SMR) is a dominant method for global hydrogen production but is associated with high carbon emissions due to its reliance on high-temperature conditions. Photocatalytic SMR is a greener and potentially more efficient alternative for hydrogen (H_2) production. Here, we present a plasmonic photocatalysis approach utilizing a Cu-Rh antenna-reactor photocatalyst, which exhibits remarkable reactivity, selectivity, and stability in SMR. The superior performance of the photocatalyst is attributed to the involvement of plasmon-mediated hot carriers. The achieved performance metrics indicate significant potential for industrial-scale implementation, and we provide suggestions for further enhancements. Notably, we observe that the catalyst displays inherent stability during photocatalysis while undergoing deactivation in thermocatalysis. Additionally, we discover the regeneration of the thermally deactivated sample through photocatalysis, and we discuss the associated mechanisms of regeneration.

OD1 – Nickel Enhances InPd-Catalyzed Nitrate Reduction Activity and N_2 Selectivity

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Nitrate (NO_3^-) and nitrite (NO_2^-) in water result from natural processes or human activities. Their harmful effects prompted the EPA to set limits of 10 mg/L and 1 mg/L as nitrogen for NO_3^- and NO_2^-, respectively, in drinking water. Bimetallic palladium (Pd) catalysts with indium (In) have been studied for removing these contaminants, but cost and availability issues hinder commercialization. To address this, we investigated replacing a significant amount of Pd with more affordable nickel (Ni) as Ni shares similar properties to Pd making it a promising alternative for thermocatalytic reduction of NO_3^-. We synthesized the activated carbon supported InPdNi/AC (0.05 wt% In, 0.3 wt% Pd, 1 wt% Ni) catalyst for nitrate reduction and compared its performance to the benchmark InPd/AC (0.05 wt% In, 1.3 wt% Pd) catalyst. Though the InPd/AC was active to NO_3^-, InPdNi/AC catalyst was ×18.3 more active. We suggest that the electron donation from Ni to Pd has been observed through X-ray photoelectron spectroscopy (XPS) and DFT calculations. This donation increases the electron density of Pd, resulting in improved removal of NO_3^-. Through CatCost analysis, we estimate that substituting 1 wt% of Pd with Ni could lead to a 70% reduction in catalyst expenses. This study opens up new possibilities for widespread commercialization of catalyst technology for nitrate/nitrite treatment by reducing the cost and usage of precious metals while enhancing catalytic activity.

OD2 – Finite Temperature Quantum Matter with Rydberg or Molecule Synthetic Dimension

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Synthetic dimension platforms offer pathways to study unique quantum matter. In this talk, we will discuss the phase diagram of a quantum many-body system of ultracold atoms (or polar molecules) with a set of Rydberg states (or rotational states) as synthetic dimension. The particles are arranged in optical microtrap arrays and interact via dipole-dipole exchange interaction. We employ mean-field theory to compute the phase diagram. We find three ordered phases – two are localized along the synthetic dimension as predicted in *Sci Rep* **8**, 3422 (2018), and a delocalized phase. We use group theoretic arguments to characterize the phases with their symmetry-breaking patterns. We will also discuss the thermal phase transitions of the system. We observe a tri-critical point on the phase boundary. Through the scaling of the tri-critical point and other special points with the number of synthetic sites, we further the knowledge for the system with thermodynamically large synthetic dimension. We will conclude with some remaining questions and other possible systems that can be explored with synthetic dimension platforms.

OD3 – Towards Sample-to-Answer HPV 16 and HPV 18 mRNA Detection for Assessing Cervical Cancer Risk

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mRNA from high-risk human papillomaviruses like HPV 16 and 18 is a highly specific biomarker for cervical cancer risk due to its ability to identify infections most likely to progress to cancer. In low-resource settings (LRS), however, where most cervical cancer cases occur, available methods for mRNA detection are inaccessible because sample preparation and detection require expensive instrumentation and highly trained users. Additionally, existing mRNA detection platforms fail to offer quantitative results, which are helpful for assessing lesion severity. Here, we describe progress towards a sample-to-answer test capable of detecting HPV 16 and 18 mRNA at clinically relevant levels with very limited equipment and few user steps. First, a one-step reverse transcription recombinase polymerase amplification (RT-RPA) assay was designed to isothermally amplify and detect HPV 16 and 18 E7 mRNA from cells from patient samples with a semi-quantitative fluorescent readout. Sample preparation involves using a combination of enzymes to lyse cells from patient samples and remove the cellular DNA, leaving the cellular RNA available for detection. A positive control assay detecting beta-actin is used to confirm sufficient genetic material for an accurate result. Second, progress has been made toward integrating sample preparation, amplification, and readout in a paper-based platform. Combined with a low-cost optical reader, the paper-based platform is expected to further reduce the equipment needed to run this test. Altogether, this test has the potential to bring more specific cervical cancer screening to LRS, permitting more efficient allocation of resources and reducing overtreatment.

OD4 – Anomalous Hall effect in the antiferromagnetic Weyl semimetal SmAlSi

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Large intrinsic anomalous Hall effect (AHE) has been considered evidence for Weyl nodes in magnetic Weyl semimetals. Compared to a normal ferromagnet, the AHE in Weyl semimetals originates from an effective field generated by the Weyl nodes, does not require a net magnetization, and should also persist in both the antiferromagnetic (AFM) and paramagnetic (PM) materials. So far, AHE has only been observed in a few AFM Weyl semimetals in magnetic field, including GdPtBi and Mn_3Sn [1,2]. Two different AHE mechanisms have been proposed in these compounds [1,3], posing a general question: what are the AHE mechanisms for other AFM Weyl semimetals?

Here we focus on another Weyl semimetal SmAlSi, and we report the observation of large anomalous Hall conductivity (AHC) (~10^2 Ohm^{-1} cm^{-1}). We propose a Weyl nodes evolution picture for the AHE in SmAlSi, different from that of GdPtBi and Mn_3Sn. Analysis of our angle-dependent quantum oscillation measurements shows strong evidence of the Weyl pockets close to the Fermi energy in both the AFM and the PM state. In this compound, the AHC increases monotonically on cooling and persists in both the AFM and the PM state up to 100 K, which is almost an order of magnitude large than the ordering temperature T_N = 11.3 K. We discuss the temperature dependence of the AHE with the proposed Weyl nodes evolution picture.

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OD5 – Kramers nodal lines in SmAlSi and other ideal candidates, (Pb/In)TaX_2 (X = S or Se)

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Kramers nodal lines (KNLs) have recently been proposed theoretically as a special type of Weyl line degeneracy that connects time reversal invariant momenta. KNLs are robust to spin-orbit coupling and are inherent to all non-centrosymmetric achiral crystal structures, leading to unusual spin, magneto-electric, and optical properties. However, their existence in real quantum materials has not been experimentally established. Here using angle-resolved photoemission spectroscopy, density functional theory calculations, and magneto-transport methods, we demonstrate the existence of KNLs in SmAlSi, a non-centrosymmetric metal that develops incommensurate spin density waves at low temperature. We further emphasize that then all the isostructural compounds in the RAlSi/Ge (R = La-Nd) material family should be hosts of KNLs. Carrying on the task of realizing ideal Kramers nodal line metals (KNLMs), we further provide experimental evidence that in the Pb/In intercalated TaX_2 (X = S or Se) material family, the KNLs cross the Fermi level and enforce the spindle-like Fermi surface touching. Due to the achiral structure of KNLMs, the lack of inversion symmetry also serves as the prerequisite of hosting Weyl fermions. In SmAlSi, we discuss whether the emergent magnetic order could originate from Weyl pocket nesting. Our combined experimental and theoretical efforts have shown a progressive pathway towards realizing ideal KNLMs in weakly-interacting and correlated materials. In the meantime, our findings provoke deeper thinking on what role topological quasiparticles should play in mediating magnetic interactions in the SmAlSi material family.

F1 – Observing an Ideal Balance: Cathode Thickness Effects on Electrochemical Performance

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Lithium iron phosphate (LiFePO4) and its derivatives are lighter and more environmentally sustainable than alternative cathode materials including LiNiCoAl and LiNiMnCo. Herein, the electrochemical performance of LiFePO4 and $LiMn_{0.6}Fe_{0.4}PO4$ cathodes of 40μm and 160μm thicknesses are investigated to elucidate the electrode thickness effects. Electrodes were prepared by casting slurry on 17μm aluminum foil and calendaring to achieve controlled porosity. CR2032 half cells are assembled and cycled in a battery tester to record rate performance. Thicker electrodes are attractive for batteries because it increases the maximum energy density at the cell level. Such improvement, however, sacrifices high C-rate performance as a tradeoff. A maximum working C-rate of 2.0 is observed for the 160μm LiFePO4 and $LiMn_{0.6}Fe_{0.4}PO4$ cathode, at which 74% and 87% specific discharge capacity (mAh/g) is retained, respectively. The results suggest $LiMn_{0.6}Fe_{0.4}PO4$ as a superior derivative of LiFePO4 for thick electrode applications. Future work will focus on intermediate thicknesses (e.g. 80 and 120 μm) to determine an optimal electrode thickness that strikes a balance between energy and power density.

P1 – Advancing Efficient CO_2 Electrolysis Systems with Resin Wafer-Based Solid Particle Electrolyte

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The utilization of chemical fuels obtained from CO_2 conversion represents a promising strategy for addressing carbon emissions. However, conventional CO_2 reduction reactors employing liquid-based electrolytes encounter challenges such as the need for additional purification steps and CO_2 crossover, leading to decreased energy efficiency. To address these issues, this study focuses on the development and performance evaluation of a solid particle electrolyte as a viable solution for overcoming the challenges associated with CO_2 electrolyzer. Specifically, sulfonated polystyrene-divinylbenzene particles were synthesized and examined as solid polymer electrolytes in CO_2 reduction electrolyzer. Through successful integration with a polysulfone binder, these particles were transformed into a resin wafer, showcasing remarkable attributes such as high ionic conductivity, low resistivity, and mechanical durability. The impedance of the solid electrolyte reactor was measured to be less than 5 Ω including electrical connections to the instrument. Using the bismuth oxide catalyst for CO2 reduction to formic acid (HCOOH), we demonstrated up to 90% Faradaic efficiency under a 200 $mA\ cm^{-2}$ current. Such findings underscore the significant potential of this research in advancing efficient and sustainable CO_2 electrolysis systems, thereby contributing to the continued progress of carbon capture and utilization technologies.

P2 – Fenton-like catalyst-incorporated ceramic membranes hybrid system for the advanced water treatment

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Advanced oxidation processes (AOPs) have been applied to mineralize the contaminants of emerging concerns (CECs) such as pharmaceuticals personal care products (PPCPs) and disinfection by-products. Among AOP technologies, Fenton-like reactions have been widely applied to get high-quality water because of the effective decomposition of H_2O_2 to hydroxyl radicals (·OH) on the surface of a heterogeneous catalyst. However, Fenton-like catalysts are critical hurdles that require activity in extremely acidic pH conditions and high-energy consumption for its recovery to be practically used. Therefore, the purpose of the study is to fabricate novel heterogeneous Fenton-like catalysts offering excellent catalytic performance under neutral pH conditions and to prepare catalyst-incorporated ceramic membranes as a continuous flow system. In this study, the rare earth-based heterogeneous catalyst was fabricated by sol-gel methods and successfully incorporated with the ceramic membrane by the pore filling and impregnation coating method. As a result, the yield of ·OH generation was enhanced by adding 20% Sm in CeO_2 (SDC) due to the increase of oxygen vacancy in activate sites. The hybrid system showed excellent performance of mineralization with over 70% of total organic carbon (TOC) removal efficiency on selected micropollutants and humic acid at 80 s of contact time (20 LMH of flux) at neutral pH. In conclusion, the Fenton-like catalyst-incorporated ceramic membranes hybrid system was successfully developed by a novel coating method, thus being an effective strategy for enhancing the efficiency of Fenton-like reaction at neutral pH conditions associated with the compact, simple, and continuous system as an advanced water treatment module.

P3 – Identifying the features that contribute to peptide-peptide synergy against E. coli using Spearman's correlation for small datasets

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With the urgent need for new medical approaches due to increased bacterial resistance to antibiotics, antimicrobial peptides (AMPs) have been considered as potential treatments for infections. Experiments indicate that combinations of several types of AMPs might be more effective at inhibiting bacterial growth with reduced toxicity and a lower likelihood of inducing bacteria resistance. The molecular mechanisms of AMP-AMP synergistic antimicrobial activity, however, remain not well understood. Here, we present a theoretical approach that allows us to relate the physicochemical properties of AMPs and their antimicrobial cooperativity. A concept of physicochemical similarity is introduced, and it is found that less similar AMPs with respect to certain physicochemical properties lead to greater synergy because of their complementary antibacterial actions. The analysis of correlations between the similarity and the antimicrobial properties allows us to effectively separate synergistic from non-synergistic AMPs pairs. Our theoretical approach can be used for the rational design of more effective AMPs combinations for specific bacterial targets, for clarifying the mechanisms of bacterial elimination, and for a better understanding of cooperativity phenomena in biological systems.

P4 – Nucleosome Breathing Facilitates the Search for Hidden DNA Sites by Pioneer Transcription Factors

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Transfer of genetic information starts with transcription factors (TFs) associating to specific sites on DNA. But in living cells DNA is mostly covered by nucleosomes, preventing access to these sites. There are conformational transformations (nucleosome breathing) that transiently open parts of DNA, but they are too fast. At the same time, there are experimental observations, indicating that some proteins, known as pioneer TFs, can efficiently reach the DNA sites hidden by nucleosomes, although the underlying mechanisms remain not understood. Using the recently proposed idea of interaction-compensation mechanism, we develop a discrete-state stochastic model for the target search on DNA with nucleosome breathing. It is found that nucleosome breathing can significantly accelerate the search by pioneer TFs in comparison to situations without breathing. We argue that this is the result of the interaction-compensation mechanism that allows proteins to enter the inner nucleosome region through the outer DNA segment that experiences frequent conformational transitions. It is suggested that nature optimized pioneer TFs to take advantage of nucleosome breathing dynamics. Our theoretical predictions agree with experimental observations for live cells. The presented theoretical picture provides a possible microscopic explanation for the successful invasion of nucleosome-buried genes.

P5 – Rapid Biomarker Screening of Alzheimer's Disease by Interpretable Machine Learning and Two-Dimensional Material-Assisted Raman Spectroscopy

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Alzheimer's disease (AD) is the most common form of dementia worldwide and is characterized by progressive cognitive decline. Rapid and accurate identification of AD biomarkers in the brain is critical to providing key insights into AD and facilitating the development of early diagnosis methods. Two-dimensional (2D) materials are at the forefront of biomedical research. In this work, we developed a platform that enables a rapid screening of AD biomarkers by employing graphene-assisted Raman spectroscopy and machine learning interpretation in AD transgenic animal brains. Specifically, we collected Raman spectra on slices of mouse brains with and without AD and used machine learning to classify AD and non-AD spectra. By contacting monolayer graphene with the brain slices, the accuracy was increased from 77% to 98% in machine learning classification. Further, using a linear support vector machine (SVM), we identified a spectral feature importance map that reveals the importance of each Raman wavenumber in classifying AD and non-AD spectra. Based on this spectral feature importance map, we identified AD biomarkers including Aβ and tau proteins and other potential biomarkers, such as triolein, phosphatidylcholine, and actin, which have been confirmed by other biochemical studies. We also investigated MoS_2 as a promising 2D material to enhance the Raman signal for biomarker detection. Our Raman−machine learning integrated method with interpretability will facilitate the study of AD and can be extended to other tissues and biofluids and for various other diseases.

P6 – Possible topological Weyl semimetal behavior in the Kondo lattice $CeRh_2Ga_2$

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Ce-based intermetallic compounds exhibit diverse magnetic states due to competing Kondo, crystal field, and Ruderman-Kittel-Kasuya-Yosida interactions [1]. Moreover, some of the Ce-based compounds have been shown to provide a rich platform for exploring the interplay between strong correlations, topology, and quantum phenomena. Particularly, $CeRh_2Ga_2$ has been theoretically identified to be a strongly correlated paramagnetic semimetal and exhibit correlation-driven topological properties [2]. In this work, we report the synthesis of $CeRh_2Ga_2$ single crystals for the first time, and present structural, magnetic, electrical transport and specific heat properties. $CeRh_2Ga_2$ crystallizes in the centrosymmetric tetragonal $CaBe_2Ge_2$-type structure (*P4/nmm*). The magnetic measurements reveal paramagnetic behavior with no evidence of long-range magnetic order down to 2.5 K. The zero field resistivity data reveal metallic Kondo lattice behavior at low temperature. The specific heat measurements yield a Sommerfeld coefficient γ = 170 $mJ/molK^2$ characterizing the compound as a moderate heavy fermion system. Surprisingly, the magnetoresistance of $CeRh_2Ga_2$ is negative in a large range of magnetic fields and temperatures, which is uncommon in a paramagnetic compound. The Hall resistivity in the paramagnetic state shows anomalous behavior which is similar to that of the established non-centrosymmetric Weyl-Kondo semimetal $Ce_3Bi_4Pd_4$ [3]. This implies a possible topological behavior in $CeRh_2Ga_2$. Our preliminary findings offer a glimpse into the realm of materials where strong correlations lead to the emergence of topological responses.

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P7 – Dynamics of single-base editing

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Recent experimental advances led to the development of DNA base editors (BEs) with a single-nucleotide precision which is critical for future progress in various scientific and technological fields. The molecular mechanisms of single- base discrimination, however, remain not well understood. Using a recently developed stochastic approach, we theoretically investigated the dynamics of single-base editing. More specifically, transient and mean times to edit ”TC” motifs by cytosine BEs are explicitly evaluated for correct (target) and incorrect (bystander) locations on DNA. In addition, the effect of mutations on the dynamics of the single-base edition is also analyzed. It is found that for most ranges of parameters, it is possible to temporarily separate target and bystander products of base editing, supporting the idea of dynamic selectivity as a method of improving the precision of single-base editing. We conclude that to improve the efficiency of single-base editing, selecting the probability or selecting the time requires different strategies. Physical-chemical arguments to explain the observed dynamic properties are presented. The theoretical analysis clarifies some important aspects of molecular mechanisms of selective base editing.

G01 – Synthesis of Al@TiO_2-Pd Nanoparticle for Plasmon Driven CO_2 Hydrogenation to CH_3OH

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Carbon dioxide (CO_2) hydrogenation to methanol is an efficient method to reduce anthropogenic CO_2 emissions and a promising route for converting CO_2 into an important chemical feedstock. Antenna-reactor plasmonic photocatalysis shows promise as a unique method to drive this selective chemical transformation. In this study, we present a Pd-decorated Al@TiO_2 core-shell nanoparticle as an efficient antenna-reactor geometry for mild-temperature CO_2 hydrogenation to methanol. In addition to the shuttle of hot carriers from plasmonic Al to the catalytic Pd nanoparticle in antenna-reactor complexes, the integration of a TiO_2 interface between Al and Pd in this new antenna-reactor geometry offers stability to the aluminum NPs and serves as a Schottky barrier that enhances the separation of energetic carriers for increased photocatalytic reactivity. This strategy prevents energetic carrier recombination and enhances the utilization of hot electrons for plasmonic CO_2 hydrogenation.

G02 – High-Precision Surgical Robot for Efficient Ultraflexible Nanoelectronic Threads Surgical Insertion

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Neural interfaces have shown remarkable potential in restoring sensory and motor function and treating neurological disorders. I present a cutting-edge surgical robot designed to revolutionize neural thread insertion, addressing the need for faster and more efficient procedures for ultra-flexible neural electrodes (NETs) surgeries. Currently, the slow and extremely limited robotic insertion methods hinder the widespread adoption of advanced brain-machine interfaces. My surgical robot is capable of simultaneously inserting 32 ultra- flexible electrode threads into wide cortical regions. Each thread contains multiple recording sites, offering potential access to over 5000 channels for data acquisition. With high-precision laser technology, needle localization accuracy reaches few micrometer to tens of micrometer range, ensuring precise placement for vessel avoidance, reducing immune response. To enhance safety, I present preliminary blood vessel detection algorithms that can later be incorporated to the surgical robot. Its user-friendly interface features pre-coded surgical procedures, streamlining the surgeon's experience and increasing procedural efficiency and control. By enhancing the efficiency and precision of neural thread insertion, our surgical robot represents a crucial advancement in brain-machine interface technology. In conclusion, our novel surgical robot offers a compelling solution to expedite and streamline ultra-flexible neural thread insertion. By combining high-precision localization, safety features, and an intuitive user interface, we believe this technology holds great promise for advancing the field of brain-machine interfaces and opening new avenues for neurosurgeons and researchers alike.

G03 – Chip-less Microencapsulation in a Bone Microenvironment for a Single-Cell Microfluidic Protein Fractionation Assay

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Despite its common use, 2D cell culture fails to model the in-vivo environment of the body thereby providing inaccurate data regarding disease morphology and progression, cell response to drugs and other processes[1]. Two-D cell culture analyses are also commonly performed on cells in bulk further convoluting information about highly diverse cell populations such as those found in tumors. Biomimicking single cell proteomics tools are necessary to better study complex diseases and further develop improved therapeutic strategies. Single cell microfluidic analysis devices such as the cutting-edge protein complex fractionation platform SIFTER[2] offer tools to study nuanced pathologies such as ES, but these devices have yet to incorporate 3D culture. Here, we present a method for the bulk fabrication of collagen 1 (COL1)-based gel microspheres encapsulating ES cells followed by incorporation of spheres with SIFTER. COL1 and hydroxyapatite (HA) were used to model an in-vivo, bone environment and introduce 3D, biomimicking cell culture to SIFTER. Neutralized COL1 supplemented with cells and/or HA was processed under agitation in oil supplemented with the surfactant Span80 to create a microemulsion thereby forming microspheres to be settled on SIFTER. We observe this method allows for sphere generation and cell encapsulation efficiency comparable to microfluidic techniques while being much less intensive. We observe SIFTER's single cell proteomics capabilities are not hindered by the addition of the bone microenvironment on-chip. To our knowledge, this work represents the first incorporation of cells in 3D models on a high-throughput single-cell protein fractionation assay while preserving the capabilities of the device.

G04 – Tailoring the properties of the surface oxide of Al Nanocrystals for specific plasmonic photocatalytic reactivities

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Aluminum in nanocrystalline form is of increasing interest as an earth-abundant optical frequency antenna for plasmonic photocatalysis. Its native surface oxide, alumina, already well-known in its pure form as a thermal catalyst, may also provide reactive sites for plasmonic photocatalytic chemistries. Here we examine how the native surface oxide of aluminum nanocrystals may be modified to become photocatalytically active as the reactor entity of an antenna-reactor complex, and how various annealing strategies can controllably manipulate its reactive properties. Annealing under different gas atmospheres changes the oxide coordination and surface morphology, enabling control of surface acidity, defect density, and carrier mobility. By modifying the surface oxide using this approach, three different aluminum-alumina antenna-reactor photocatalysts can be realized, with native oxides tailored for different types of chemical reactions.

G05 – Optimizing Feature Selection and Hyperparameters in Machine Learning for Improved Single Particle Trajectory Classification.

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Diffusion is a fundamental process with significant implications in diverse fields such as drug delivery, protein-protein interaction, and the food industry. However, accurately characterizing different modes of diffusion poses challenges, particularly when dealing with short and noisy trajectories observed through single particle tracking (SPT) experiments. To overcome this challenge, in this study, artificial intelligence (AI) methods have been harnessed to enhance the characterization of single particle trajectories. Feature selection algorithms have been employed to identify the most influential features for precise trajectory characterization. Consistently across all algorithms, the top three features identified are Efficiency, Fractal Dimension, and Trappeddness, indicating their crucial roles in characterizing single particle motion. To assess the impact of these features, a comparative analysis of model accuracy is conducted between the base model utilizing all nine features and models incorporating the top three features from each algorithm. The results reveal that the model employing the Neighborhood Component Analysis (NCA) algorithm achieves the highest accuracy at 70.52%. To further enhance the model's accuracy, various hyperparameter tuning methods are implemented. Among which, Random Search proves to be the most effective, attaining an accuracy of 81.66%. Additionally, K-fold cross-validation is employed on the Random Search model, leading to the identification of the best-performing model. Overall, this research contributes to the advancement of single particle trajectory characterization through the utilization of feature selection algorithms, optimization techniques, and machine learning approaches ultimately facilitating improved comprehension and control of particle motion.

G06 – Understanding the Relationship between Electrochemical Fouling Control and Electrode Surface Coverage

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Electrically conductive membranes can initiate electrochemical reactions to effectively degrade or detach foulants from the membranes. This in-situ fouling control could reduce the need for backwashing fouled membranes or adding chemicals, cutting down operating costs by about 33%. Electrically conductive membranes also prevent foulants from building up on the surface, decreasing the need for pretreatment processes. Electrically conductive membranes are typically prepared by completely covering polymeric substrates with conductive materials like carbon nanotubes, but this can decrease permeability compared to pristine membranes. There is also a limited understanding of how the distribution of conductive materials on the membrane surface affects fouling control.

This study investigates the effect of partial electrode coverage on fouling control. We prepared samples with varying electrode coverages (38-100%) by laser-scribing graphitic electrodes on a polyimide substrate and then fouled them with a stable bacterial biofilm. During defouling tests, the fouled electrodes were subjected to negative or positive voltages and the specific energy consumption was measured. The results showed that full electrode coverage is not necessary to achieve complete biofilm removal, as 53% electrode coverage was found to be equivalent to biofilm removal levels of higher coverage. Additionally, partial electrode coverage required less energy for biofilm removal compared to full coverage. Notably, the developed current density under a cathodic potential of -2.5 V did not correlate with biofilm removal, suggesting that electrode morphology plays a crucial role in fouling control.

G07 – Energy-Efficient Gram-Scale Solid-State Synthesis in a Flash

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Sustainable manufacturing that prioritizes energy efficiency, minimal solvent usage, and high scalability is critical. Herein, we introduce a non-equilibrium synthesis technique called flash-within-a-flash Joule heating (FWF) as an efficient indirect Joule heating method to overcome the limitation of conductivity requirements in flash Joule heating processes (FJH). The FWF process involves using an outer vessel filled with a conductive carbon feedstock and an inner flashing vessel containing the target reagents. While FJH transforms the outer conductive carbon into turbostratic graphene, the inner reagents react due to the thermal conduction of Joule heating to form various compounds of interest. The versatility of the FWF process was demonstrated in the synthesis of various inorganic compounds with 12 transition metal dichalcogenides (TMDs) and 10 non-TMD materials serving as a universal synthesis technique that meets the modern synthesis requirements. The demonstration of doping and ease of scaling into gram-scale suggests that this method could facilitate research and industrial scale production. The field effect transistors from as-synthesized TMDs were fabricated and demonstrated outstanding electrical performances. In summary, the FWF process offers efficient and scalable routes for inorganic material synthesis enabling faster reactions, reducing environmental impacts, and providing flexibility paving the way for sustainable manufacturing processes.

G08 – Solutions are the Problem: Ordered 2D Covalent Organic Framework Films by Chemical Vapor Deposition

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Covalent Organic Frameworks (COFs) are a class of highly porous crystalline polymer networks made from two precursor monomers. They can be tailormade to have specific pore size, morphology, and functional groups based on geometry matching of their monomers. However, conventional methods of producing COFs often produce insoluble powders that require hours to days to produce. In this work, we report a chemical vapor deposition approach to produce highly crystalline and uniform thin films of three separate COF chemistries. This all-in-one synthesis technique produces highly crystalline 40 – 1000 nm thick films on a Si/SiO_2 substrate in less than 30 minutes. Using a combination of grazing-Incidence wide-angle X-ray scattering (GIWAXS) and transmission electron microscopy (TEM), we showcase high crystallinity and planar orientation of COF films. Raman, UV-Vis, and AFM have also been conducted to further show the quality of the COF film. For future work, this technique will be applied to a large variety of applications enabled by the creation of a variety of COF chemistries each with unique pore sizes, functional groups, and optical properties. These applications include hydrophobic coatings, heterogenous catalysis, nanofiltration, and more.

G09 – HF-free patterned glass enables generalizable micron-scale 3D contact printing (3DμCP)

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Microcontact printing (μCP) is a widely-used technique for biomolecule patterning using patterned polydimethylsiloxane (PDMS) stamps coated with bio-ink.[1] While μCP has various applications, its 2D limitation restricts its potential uses, particularly for 3D cell immobilization and high-throughput force microscopy. Recently, 3DμCP methods have emerged, but they typically require specialized substrates that limit printable biomolecules.[2,3] We present a novel 3DμCP method to pattern micron-scale 3D features into a glass substrate for protein contact printing. This method is generalizable to most other contact-printing and passivation protocols, which are often designed for use on glass slides. Furthermore, glass-cleaning protocols enable frequent re-use.

The process uses electron beam lithography to pattern features with <100 nm resolution on a glass slide coated with positive-tone PMMA resist. Then, reactive ion etching (RIE) using CF4 anisotropically etches channels into glass, and a subsequent oxygen RIE treatment removes excess PMMA and reconverts the now-fluorinated surface to native silicon dioxide. Critically, our method does not use highly lethal hydrofluoric acid, a traditional glass etchant. We successfully demonstrated this method on glass slide fragments in duplicate, patterning a ~2 cm^2 area with Rice owls and microposts containing 0.5-~10 micron-sized features. Brightfield microscopy indicated pattern fidelity for all features above 1 micron, and stylus profilometry showed feature depth of 40-60 nm. Contact printing using a planar PDMS stamp inked with human albumin confirmed protein adhesion to non-etched areas.

In conclusion, our method provides a versatile and safe approach for 3D protein patterning on glass substrates, broadening potential μCP applications.

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G10 – Developing a Technique to Probe Ligand Bilayer Dynamics on Au Nanoparticle Growth via Nuclear Magnetic Resonance (NMR)

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Numerous properties of inorganic nanoparticles depend on the chemical availability of the surface facets, which is largely dictated by the kinetics and thermodynamics of the ligands that can coordinate, and passivate, the nanoparticle surface. However, there is not a clear mechanistic picture of this crucial ligand behavior at nanoparticle interfaces. To better understand each of the complicated processes involved with ligand movement near the nanoparticle surface, including intra- and inter-bilayer exchange, this work aims to develop molecular characterization techniques capable of determining he location and movement of ligands relevant to the nanoparticle-bound bilayer. More specifically, this work employs the use of atomically well-defined Au_{32} nanoclusters, which can be characterized using traditional molecular techniques while still maintaining important nano-specific properties. As such, nuclear magnetic resonance spectroscopy (NMR) is used to probe the position of surface ligands with respect to the nanoparticle surface. This work suggests that by improving the synthesis of the model nanoparticle and using a combination of ^{1}H and ^{31}P 1D and diffusion ordered spectroscopy NMR, it is possible to determine whether ligand monomers are present at the nanoparticle surface or in a micellar phase in solution. In developing a method to measure surface ligand location and exchange, this work will enable the ability to determine the thermodynamic and kinetic properties of nanoparticle-bound surfactant bilayer systems, thus allowing for better control over nanoparticle syntheses.

G11 – Impregnation of KOAc on $PdAu/SiO_2$ causes Pd-acetate formation and metal restructuring

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Potassium-promoted, silica-supported PdAu is catalytically active for the gas-phase acetoxylation of ethylene with acetic acid to form vinyl acetate monomer (VAM). Potassium, which is incorporated into the catalyst via wet impregnation of its salt solution, is known to improve long-term activity and selectivity for VAM. This common catalyst preparation step is generally assumed to have no effect on catalyst structure. However, in this work, we report evidence to the contrary. We initially synthesized a silica-supported PdAu model catalyst containing Pd-rich PdAu alloy and pure Au phases. A Design of Experiments (DOE) approach was implemented to impregnate the as-synthesized $PdAu/SiO_2$ catalyst with varying loadings of potassium acetate using wet impregnation solutions with varying concentrations of acetic acid. Samples were then characterized to detect changes in metal nanoparticle structure (XRD, XPS, and XAS) and surface species formation (DRIFTS). Impregnation with KOAc aqueous solution revealed no XRD-detectible changes to the bimetal structure, whereas DRIFTS indicated the presence of $Pd_3(OAc)_6$, which led to up to 2% Pd loss after washing with water. Carrying out the impregnation step with an AcOH-only solution caused significant enlargement of the pure Au phase and generated less $Pd_3(OAc)_6$. During co-impregnation of AcOH and KOAc, grain sizes were enlarged slightly, and substantial amounts of $K_2Pd_2(OAc)_6$ and $Pd_3(OAc)_6$ were detected by DRIFTS and correlated to up to 32% Pd loss after washing. Multivariate analysis confirmed the effects from KOAc and AcOH were statistically significant. Ultimately, these results indicate wet-impregnation-induced metal leaching and restructuring can occur during catalyst preparation.

G12 – Unusual Oxidation Behavior of Aluminum Nanocrystals

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Due to increasing interest in their optical properties, the synthesis of Al nanocrystals has seen significant development over the last 10 years. Highly crystalline and pure nanoparticles have been demonstrated with varied shape and size, markedly different from the Al nanopowders produced through conventional means such as electrical explosion of bulk metal. Additionally, there is significant interest in Al nanoparticles due to their capacity for both energy release on oxidation and hydrogen release on reaction with water. To best incorporate these particles into applications, however, it is vital to understand their oxidative reactivity, and how this reactivity is impacted and controlled by the distinct sizes, crystallinity, and morphologies that can now be obtained**.** Previous work on studying the oxidation of Al nanoparticles was performed on heterogeneous and polycrystalline powders, and how the oxidation of Al nanocrystals, especially those with exotic shapes, compares to these previously studied powders is not known.

In this work, the oxidation of cubctahedral Al nanocrystals and of branched Al nanowire clusters is studied and contrasted. Thermogravimetric analysis is used to examine the oxidation on heating and shows clear size dependence, subtle changes to the oxide layer based on synthesis conditions, and an anomalously large amount of oxidation at lower temperatures for branched nanowire clusters. TEM and SEM microscopies are used to examine the particle morphologies at different stages of oxidation in order to understand the mechanisms leading to the enhanced oxidation at low temperatures, including through direct comparison of the same particles before and after oxidation.

G13 – Stimuli-responsive Gating of Single Plasmonic Nanohybrids

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Stimuli-responsive materials have attracted considerable attention due to their ability to react to external triggers. Plasmonic nanohybrids incorporating both gold nanoparticles and stimuli-responsive materials can enable the active control of plasmonic properties such as resonance tuning, charge transfer, and plasmon energy transfer. However, the broad application of plasmonic nanohybrids requires a deep understanding of the underlying mechanisms that govern their active control and responsiveness. In this work, we report the effect of polymer conformational changes on the localized surface plasmon resonance (LSPR) of single hybrid nanostructures consists of poly(*N*-isopropylacrylamide) (pNIPAM) encapsulated gold nanoparticles (AuNPs). To achieve this objective, single-particle dark-field hyperspectral imaging was used for the real-time monitoring of stimuli-modulated hybrid nanoelectrode charging via changes in the plasmon resonance. Upon changes in temperature, the resonance energy and scattering intensity show responses that are both dynamic and reversible, thus demonstrated the active control of plasmonic properties at the nanoscale. Furthermore, our single-particle approach uncovered internal heterogeneity of the plasmonic nanohybrids, which shows great promise in the understanding of structural-spectral relationship that traditional ensemble techniques are unable to discern. In conclusion, this work provides an understanding of the influence of the plasmonic core on polymer collapse dynamics, thereby enabling the rational design of flexible and easily processable devices and architectures.

G14 – Quantum Simulation of a One-Dimensional Luther-Emery Liquid

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We investigate the one-dimensional behavior of attractively interacting spin-1/2 fermions in optical lattices. With repulsive interactions, the continuum model as described by the Tomonaga-Luttinger theory has low energy excitations characterized by bosonic charge and spin excitations that propagate with different velocities. With attractive interaction, however, one expects pairing that leads to a gap in the spin sector, thus inducing decay in the spin correlations- as explained by the Luther-Emery theory. This paradigm is known to be a potential 1D analog of superconductors. We use a 2D optical lattice to realize an array of quasi-1D tubes. The tubes contain a pseudo-spin-1/2 system consisting of the lowest and third-to-lowest hyperfine sublevels of 6Li. We tune the interspecies interactions with a magnetic Feshbach resonance and use radiofrequency (RF) spectroscopy to probe dimer formation in the attractively interacting liquid. Furthermore, we implement Bragg spectroscopy to obtain low-energy excitation spectra for the charge and spin modes. Our work aims to better understand the equivalent of the "BCS-BEC crossover" in 1D.

G15 – Generating Nanometer-sized Polymer Wires with SEM/FIB Instrumentation

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Polymer fibers have great potential for various applications, such as 3D printing, biocompatible fibers, and flexible electronics and sensors [1-3]. While several methods exist for fabricating polymer fibers, including electrospinning, fiber drawing, and template-based methods, creating isolated polymer wires with dimensions in the nanometer range remains a challenge. Here, we introduce a new approach for generating polymer nanowires using FIB/SEM instrumentation. Our method enables ultralong polymer nanowires with an aspect ratio of 500:1 and a diameter of less than 1 micron. Moreover, our approach allows for in-situ visualization of the nanowire formation process in SEM with nanometer resolution, providing a better understanding of the process and underlining mechanism.

Different from the most common applications demonstrated by traditional FIB/SEM instrumentation, we utilized the tool in an innovative way. Specifically, we used the sharp OmniProbe manipulator in a ThermoFisher Helios as a needle to extract polymer wires from an isophorone diisocyanate (IPDI) monomer solution (Fig. 1a-c). Initially, we found that drawing the monomer solution does not result in long and uniform polymer fibers (Fig. 2a). To solve the problem, we fabricate IPDI solution in sealed microcapsules [4], which protected the IPDI solution and allowed for OmniProbe to access fresh IPDI solution. Fig. 1b shows an SEM image at the beginning of nanofiber drawing. Fig. 1c shows that the nanofiber can form up to 0.2 mm in length while maintaining a diameter of only ~1 micron.

Additionally, we discovered that the viscosity of the monomer solution plays a significant role in nanowire formation (Fig. 2b-d). For IPDI, a concentration of 12.5 wt% gives the ideal viscosity for nanowire formation.

Through this study, we demonstrate a novel application using FIB/SEM instrumentation for the polymer fiber research field. The approach involves using microcapsules as carriers to facilitate the fabrication and in-situ nanometer characterization of polymer wire formation in FIB/SEM. In addition to IPDI, the method can be extended to other types of polymers, such as conductive polymers. Our approach will also aid researchers in gaining a deeper understanding of the fundamental knowledge in the field of nanofibers and, ultimately, provide insight into how to engineer nanofibers for various applications.

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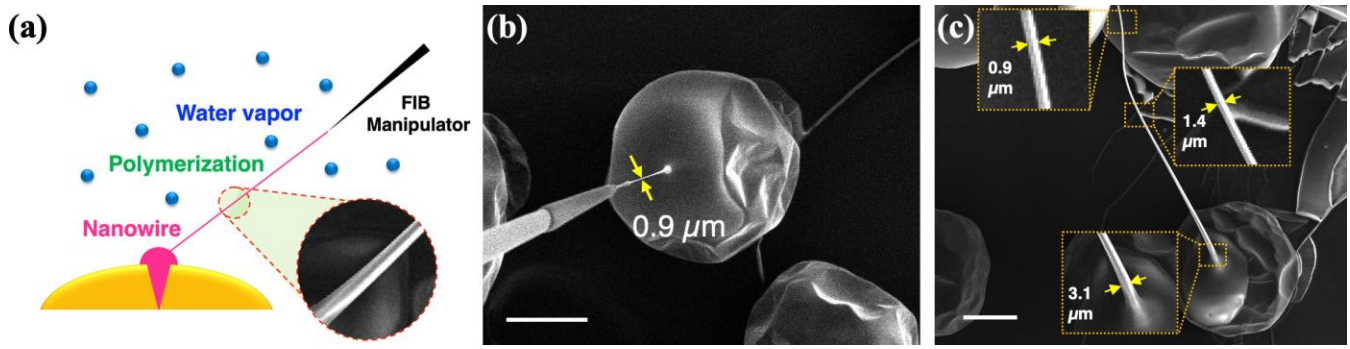

Figure 1. a, Schematic of the process for generating IPDI polymer nanowires using the OmniProbe manipulator in FIB/SEM instrumentation. **b,** SEM image of a polymer nanowire at the beginning of the drawing process. **c,** SEM image of an ultralong nanofiber drawn from the microcapsule, with labeled diameters. Scale bars in **b** and **c** are 25 μm**.**

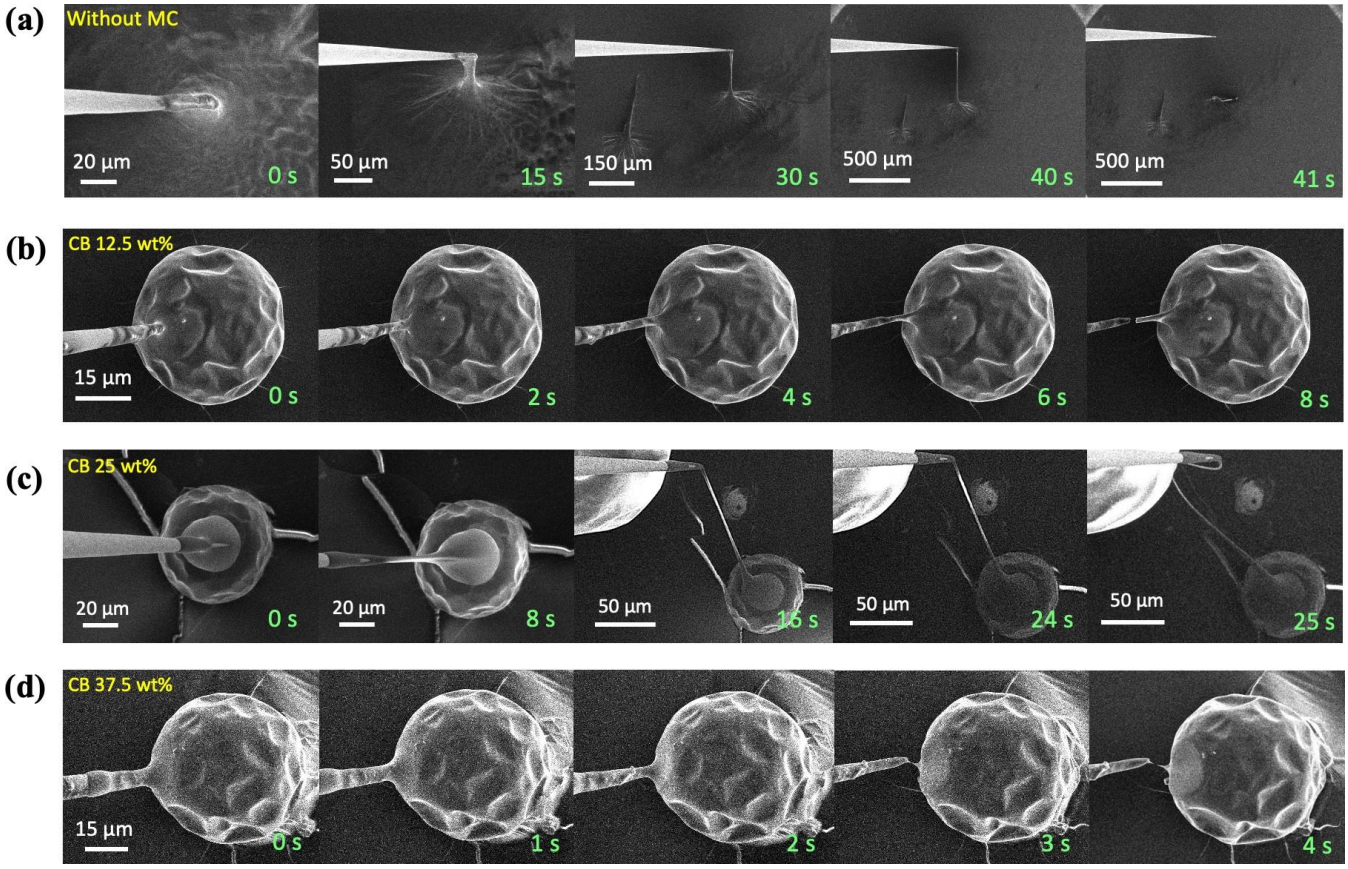

Figure 2. In-situ SEM imaging of polymer nanowires with different solution viscosity. a, Drawing wires from pure IPDI monomer solution (5g of chlorobenzene) without microcapsule container. **b-d** Drawing wires from IPDI monomer solution with the 12.5 wt% (b), 25 wt% (c), and 37.5 wt% (d), respectively. The optimized condition is 25 wt%.

G16 – Magnetospectroscopic Evidence for the Magnonic Superradiant Phase Transition in Erbium Orthoferrite

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The superradiant phase transition (SRPT) occurs when the strength of the cooperative coupling of an ensemble of two-level atoms with a bosonic excitation exceeds a critical value, creating a new ground state that possesses a finite atomic polarization with concomitant boson condensation. Photonic SRPTs have been realized only in nonequilibrium situations. Recently, a magnonic SRPT has been theoretically demonstrated for erbium orthoferrite, ErFeO3, in thermal equilibrium. This material consists of two subsystems: (i) Er3+ ions, which can be viewed as an ensemble of two-level atoms, and (ii) Fe3+ ions with magnons, which are bosonic excitations. Ultrastrong coupling between the two subsystems causes a SRPT, inducing condensation of Fe3+ magnons and an Er3+ spin polarization. Here, we provide experimental evidence for the phase transition through GHz magnetospectroscopy. We varied the detuning between the lowest Er3+ atomic transition and the Fe3+ magnon excitation via an applied DC magnetic field. This process is equivalent to the threshold modulation of the Er3+–Fe3+ coupling strength for the SRPT, which allows us to measure a rapid decrease of the resonance frequency of Er3+ spins as the system crosses the superradiant-to-normal phase boundary. Our measurements relied on minute temperature changes of an ErFeO3 crystal owing to spin–lattice coupling, by which we were able to precisely monitor peak positions as a function of magnetic field.

G17 – Title: Effective magnetic fields from chiral phonons in rare-earth halides

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Time-reversal symmetry (TRS) is pivotal for materials' optical, magnetic, topological, and transport properties. Chiral phonons, characterized by atoms rotating unidirectionally around their equilibrium positions, generate dynamic lattice structures that break TRS. Here we report that coherent chiral phonons, driven by circularly polarized terahertz light pulses, can polarize the paramagnetic spins in CeF_3 like a quasi-static magnetic field on the order of 1 Tesla. Through time-resolved Faraday rotation and Kerr ellipticity, we found the transient magnetization is only excited by pulses resonant with phonons, proportional to the angular momentum of the phonons, and growing with magnetic susceptibility at cryogenic temperatures, as expected from the spin-phonon coupling. The time-dependent effective magnetic field quantitatively agrees with that calculated from phonon dynamics. Our results may open a new route to directly investigate mode-specific spin-phonon interaction in ultrafast magnetism, energy-efficient spintronics, and non-equilibrium phases of matter with broken TRS.

G18 – Analysis of High Frequency (GHz) Gravitational Wave Detectors and New Prospect with Metasurface

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Gravitational waves, or propagating distortions in spacetime, originate from a variety of coherent and stochastic sources, ranging from astrophysical systems like black hole binaries to evolutionary processes from the early universe such as inflation, phase transitions, and cosmic strings. The first direct detection of gravitational waves was in the sub-kHz frequency range at LIGO in 2016, generated by the merging of two black holes. More recently, nanoGrav has released a 15-year dataset exhibiting a stochastic background in the nHz frequency range using the correlations between pairs of "blinking" pulsars. Interferometric methods, however, lose sensitivity at higher frequency ranges due to weaker theoretically expected perturbations. A more promising method has been studied over the past two decades, involving the detection of electromagnetic field perturbations generated by gravitational waves at microwave frequencies. The experiment consists of a static magnetic field and an AC EM field as the background fields. A high frequency gravitational wave (HFGW) passing through the detector can distort the fields and give rise to a perturbative photon flux, which can then be measured with single photon detectors in the GHz regime. The external and inherent noise in the experimental design will be analyzed, revealing sources that may overwhelm the weak signal, leading to a proposal of novel metasurface projects that may mitigate some of the issues and hope to achieve higher sensitivity.

G19 – Towards Simulating a Dissipative Quantum Phase Transition using Trapped Ions

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Dynamics in open quantum systems is defined by the competition between unitary evolution and non-unitary operations, like measurements and/or interaction with the environment. Recent theoretical studies (Sierant,2022, Quantum,6,638) in the field have predicted the existence of a dissipative phase transition (DPT) in a periodically driven-dissipative, long-range interacting quantum spin chain between a ferromagnetic ordered phase and a paramagnetic disordered phase as a function of resetting probabilities after coherent evolution. We can probe this driven-dissipative out-equilibrium dynamics using our trapped ion quantum simulator. To do so, we have developed a high optical access vacuum chamber which houses a linear, three-dimensional, blade trap to confine chains of Yb^+ ions. Using our 0.3 NA and 0.6 NA re-entrant windows, we realize global, tunable Ising type interactions (coherent) to couple spins with counter-propagating Raman beams and site-resolved dissipation (resetting) with local optical pumping (LOP) beams, respectively. We report on the latest developments in the calibration and minimization of the ion-ion crosstalk of the $< 2\mu$m waist LOP beam/ion. We further discuss the LOP scheme's ability to prepare arbitrary product states and its versatility to achieve unexplored quantum many body physics beyond DPT using our simulator.

G20 – An Assessment of BN+TiO_2 Physical Mixture for Photocatalytic Degradation of Perfluorooctanoic acid.

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Titanium dioxide (TiO_2) has been proven to be an active photocatalyst for the destruction of per- and polyfluoroalkyl substances (PFAS), a group of virtually non-destructive and persevering contaminants, commonly referred to as "forever chemicals" in regards to the stability of their C-F bonds. Despite being active, however, its activity is limited to be an effective PFOA treatment option. We have previously demonstrated that PFOA destruction was significantly enhanced by calcining TiO_2 nanopowder with hexagonal boronitride (h-BN), another effective photocatalyst. In this study, we investigated a simpler method of improving photocatalytic performance of TiO_2 by physically mixing TiO_2 nanopowder with ball-milled hexagonal boron nitride (BN) nanopowder. After 2 hours of UV-C (i.e., 254 nm) irradiation, BN + TiO_2 physical mixture was able to degrade ~ 70% PFOA. Further scavenger experiments demonstrated the presence of photogenerated holes and their role in photo-oxidation of PFOA at the ppm level. Additional experiments determined the effects of environmentally relevant conditions (e.g., salt concentrations, pH, initial PFOA concentration) on PFOA degradation. These findings motivate continued efforts in developing better photocatalysts that will make photocatalysis a viable option for sustainable, energy-efficient destruction of PFAS compounds.

G21 – Tunable Mid-IR Plasmonic Properties of SiO_2@Al-doped ZnO Particles

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Plasmonic materials (especially noble metals) have attracted significant interest due to their enhanced interactions with light at the nanoscale and the excitation of free carriers at the metallic surfaces at **short wavelengths** with diverse applications in sensing, imaging, photocatalysis and energy conversion. It is important to note, however, that plasmonics has many potential applications at **longer wavelengths** as well, specifically, the mid-infrared wavelength range (3-30um), characterized by strong and distinct vibrational and rotational absorption peaks of many molecules, and which are also the peak areas for blackbody emission for most biological and mechanical objects, resulting in design and fabrication of more nuanced optical and thermal sensors.

Recent studies have shown that conductive metal oxides are good candidates for low energy plasmonics due to their lack of interband transitions in the mid-IR. This work, through a combination of theoretical simulations and synthesis development, explores the synthesis and plasmonic properties of SiO_2@Al-doped ZnO (AZO) core-shell nanospheres. The synthesis of these particles is developed, allowing for tunable post-annealing shell thicknesses greater than 100 nm and widely tunable Al doping. The effects of doping concentration, particle size, and interparticle distance are explored theoretically with Mie theory and the finite element method and can now be examined experimentally as well.

G22 – Cluster-based methods for strongly-correlated spin systems

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Strongly-correlated systems, such as iron-sulfur clusters, conjugated hydrocarbons, and superconductors, pose significant challenges in quantum many-body physics and chemistry. Here, we present two novel approaches based on cluster mean-field theory (cMF) to tackle the ground-state description of such systems. The main ingredient of cluster-based methods is tiling of the system, which is performed using the proximity of sites in real space. The first approach employs an unrestricted cluster mean-field framework (UcMF) with each cluster being an S_z eigenstate. Due to this framework's simplicity, correlated methods based on perturbation theory (cPT2) and coupled-cluster (cCCSD) are subsequently used to account for the missing inter-cluster correlations. In the second approach, we introduce the generalized cluster mean-field theory (GcMF), which allows S_z to break in each cluster. By relaxing this condition, each cluster is allowed to access all S_z sectors, thereby partially incorporating missing correlations. Improving the method further, we employ a projection scheme to restore the global S_z symmetry, resulting in the spin-projected generalized cluster mean-field method (S_zGcMF). Benchmark calculations on the one- and two-dimensional XXZ and J_1-J_2 Heisenberg models demonstrate the accuracy and reliability of the proposed methods. More specifically, GcMF and S_zGcMF can qualitatively capture correlations that are missing in UcMF and present a better alternative as a reference method, whereas cPT2 and cCCSD applied on UcMF can quantitatively capture the inter-cluster interactions for some systems. Overall, our findings indicate that cluster-based methods are useful tools for studying strongly-correlated spin systems and present potential for further development.

G23 – Unveiling Complex Magnetic Behavior in Gd_5Pb_3

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The intermetallic R_5Pb_3 (R = rare earth) family of compounds crystallize in a hexagonal $P6_3/mcm$ structure, where the rare earth ions are located at two inequivalent crystallographic sites. These compounds are therefore expected to display complex magnetic ordering due to the different coupling between the two different magnetic sublattices leading to anisotropic exchange. Thus far, characterization studies have only been done on polycrystalline samples of this family. We have synthesized single crystals of Gd_5Pb_3 and performed magnetization, electrical transport, and specific heat measurements on them. We find that Gd_5Pb_3 orders ferromagnetically close to room temperature, which is unusual for a rare-earth based magnet, and displays complex magnetic behavior upon cooling down to lowest temperatures. In-plane and out-of-plane magnetic measurements reveal high anisotropy, which cannot be attributed to crystal field effects. Thus, our results provide a solid basis of experimental observations to motivate further studies to understand the complex anisotropic exchange occurring in Gd_5Pb_3 as well as gain insight into the behavior of rare-earth based intermetallic R_5Pb_3 family of compounds.

G24 – Terahertz Chiral Optics with Ordered Carbon Nanotube Architectures

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Electromagnetic waves in the terahertz (THz) frequency range, from 0.1 to 10 THz, have garnered great interest due to their diverse potential applications in spectroscopy, quantum electronics, sensing, and wireless communications beyond 5G. One crucial capability for various applications is efficiently manipulating polarization states of THz waves. Previous work utilizing aligned carbon nanotube (CNT) films fabricated by the controlled vacuum filtration method [1] has demonstrated remarkable polarization rotations, with transmitted THz pulses showing rotations of up to 20 degrees and reflected pulses exhibiting rotations of up to 110 degrees [2]. Here, we employed two methods for creating macroscopically ordered CNT assemblies with synthetic chirality for manipulating circular polarization states of THz radiation. Both methods resulted in wafer-scale chiral CNT architectures that demonstrated tunable and giant circular dichroism [3]. These approaches, (i) mechanical rotation and (ii) twist-stacking, utilize controlled vacuum filtration to create circular patterns of CNTs or stack linearly aligned CNT films at a twist angle to each other. Our THz transmission spectroscopy experiments exhibited values of circular dichroism up to 6 degrees in ultrathin (~30 nm) films, showing that these macroscopic chiral structures hold great potential as THz modulators.

[1] X. He *et al*., 2016, *Nature Nanotechnology*, *11*, 633–638;

[2] A. Baydin *et al*., 2021, *Optica*, *8*, 760;

[3] J. Doumani *et al*., 2023, *Nature Communications*, under review.

G25 – Surface-Enhanced Vibrational Spectroscopies for the Detection of Polycyclic Aromatic Compounds

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Polycyclic aromatic hydrocarbons (PAHs) are a class of environmental contaminants with known carcinogenic effects. Derivatized PAHs, known as polycyclic aromatic compounds (PACs), containing oxygen, sulfur or nitrogen functional groups, frequently manifest similar or higher toxic and mutagenic effects as their PAH analogs. A promising avenue for rapid, more accessible chemical detection is that of plasmon-based surface-enhanced spectroscopies. Surface-Enhanced Raman Scattering (SERS) and Surface-Enhanced Infrared Absorption (SEIRA) can be used for the ultrasensitive detection of chemical species, enabling limits of detection as low as parts-per-billion in many cases, and even single-molecule sensitivities. Using substrates consisting of aggregated gold nanoshells (GNS), capable of enhancing both SERS and SEIRA, we studied the detection of PACs. Focusing on anthraquinone, nitroanthracene, tetracenequinone, and nitropyrene as model PAC contaminants, we demonstrate SEIRA-based chemical detection. The particles were functionalized with self-assembled monolayers of 11-mercapto-1-undecanol (MUO). The adsorption of PACs is facilitated by intermolecular interactions between the functional groups of the analytes and the terminal hydroxyl groups on the surface. The interactions can be observed in the SEIRA spectra of the captured PACs, which agree well with density functional theory calculations. Additionally, we show the capacity to do computational separation of spectral signal sources based on multiple SEIRA spectral measurements.

G26 – Thermal imaging through hot emissive windows

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Enhancing thermal emission in a specific direction while suppressing it in the rest is a complex problem, especially when such a directional emitting device must also remain fairly transparent in the same spectral window. This complex problem has haunted applications such as thermal imaging through a hot emissive window where emission from the hot window can be strong enough to blind the camera. Here, we demonstrate a solution to this problem and enable thermal imaging through hot windows. We show that an engineered nanostructured coating on a window at 873 K suppresses thermal emission toward the camera while maintaining fairly good transmission to allow thermal imaging through it. The nanostructured coating employs asymmetric spatial distribution of absorption losses in nanoscale resonators to achieve the desired functionality. While resonance enhanced temporal coherence, the asymmetric loss distribution enabled directional emission at the cost of some transmission through the window. Our asymmetrically emitting window enhanced the thermal imaging contrast by nearly 2.4 times when held at 873K when compared to a conventional window.

G27 – Raman Spectroscopy of Chiral Carbon Nanotube Architectures with Circularly Polarized Light

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Using polarization-dependent Raman spectroscopy, we have probed the structure-induced chiral behavior of aligned and twisted single-wall carbon nanotube films prepared by controlled vacuum filtration. We found that the intensity of the G-band sensitively depends on the relationship between the sense of circular polarization of the excitation beam and the handedness of the chiral carbon nanotube architecture under study, thus allowing us to easily differentiate between left- and right-handed stacked films. This study therefore presents circularly polarized Raman spectroscopy as a powerful and convenient tool for studying chiral matter, as an alternative to the commonly used circular dichroism spectroscopy.

G28 – Towards Analog Quantum Simulation of Three-Body Hamiltonians with Ytterbium Trapped Ions

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Trapped ion qubits provide a reliable platform for the analog simulation of quantum spin systems because of their high controllability, scalability, and long coherence times. The mapping of quantum field theories to spin models further enables us to study condensed matter, nuclear, and high energy physics with trapped ions. We will report our experimental progress towards an analog quantum simulator with a trapped Ytterbium ion chain, including the characterization of our trap performance and its stability. Here, we also propose the generalized Molmer-Sorensen scheme using higher order spin-phonon couplings to generate an effective three-body Hamiltonian with trapped ions, which would allow us to simulate the U(1) quantum link model. Furthermore, we will present our individual addressing setup using an arbitrary wave generator and a free-spaced acoustic optical-modulator for local optical pumping. This configuration will be used for spin state initialization, which is necessary to characterize the dynamics of the three-body Hamiltonian.

G29 – Characterization of Guanine Functionalized SWCNTs by Raman Spectroscopy

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Single-walled carbon nanotubes (SWCNTs) have peculiar optoelectronic properties that render them an important class of materials for future nanoelectronics and bio-nano sensors applications. It was recently discovered that it is possible to spatially modify the SWCNTs bandgap and thereby modulate their electronic and optical properties in a controlled manner by Guanine functionalization reaction.[1] This happens through exposing SWCNT coated by single-stranded DNA to singlet oxygen, which results in the covalent bond formation between the guanine nucleobases in the DNA coatings to the nanotube sidewalls.

Spectroscopic tracking of the extent of guanine functionalization is mostly done by Raman and Fluorescence spectroscopy. The ratio of D-band to G-band in the Raman spectra is commonly used as a measure of sp3 defects effected by guanine functionalization; however, this method is suffering from the fact that is not possible to distinguish between different SWCNTs chiralities for an unsorted sample. The fluorescence spectra of functionalized SWCNTs shows red shift and broadening compared to the pristine sample. This broadening makes deconvolution of the spectrum of a sample with a mixture of several SWCNTs chiralities imprecise.

Here we will demonstrate that upon guanine functionalization reaction a new Raman band arises that allows for a novel chirality-selective method to monitor the degree of guanine functionalization. In addition, we will describe our understanding of the nature of this band.

1. Zheng, Y.; Bachilo, S. M.; Weisman, R. B., Controlled patterning of carbon nanotube energy levels by covalent DNA functionalization. *ACS Nano* **2019,** *13,* 8222-8228.

G30 – Phonon ray tracing calculations of ballistic temperature and heat flux profiles in nanostructures

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Phonon ray tracing calculations have been used to quantify phonon boundary scattering in nanomaterials and to interpret thermal conductivity measurements. However, these phonon ray tracing method have not been able to access the temperature or heat flux profiles within nanomaterials, making it difficult to gain insight into the ballistic transport physics or to model nanoscale temperature mapping experiments using phonon ray tracing. Here, we derive and apply phonon Monte Carlo ray tracing methods to calculate these local temperature and local heat fluxes in semiconducting nanomaterials, with a focus on the ballistic transport regime. The derivation provides a straightforward interpretation of the local temperature in terms of a thermal conductance ratio, and the local heat flux in terms of the difference between forward- and reverse-oriented phonon trajectories crossing a control surface. After validating the method for different transport regimes and geometries, the ray tracing results are used to optimize geometric parameters to enable locally inverted temperature gradients in porous nanomeshes, and to evaluate the heat focusing capabilities of geometric ballistic phonon lenses. These applications illustrate how phonon ray tracing methods can be used to quantify ballistic thermal profiles and to design porous nanostructures that exhibit atypical thermal behaviors in the ballistic regime.

G31 – Surface Functionalization of Aluminum Nanocrystals for SERS

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Polycyclic Aromatic Hydrocarbons (PAHs) are ubiquitous pollutants that bind with DNA to form carcinogenic adducts. Plasmonically enhanced sensing strategies such as Surface Enhanced Raman Scattering (SERS) and Surface Enhanced IR Absorption (SEIRA) can detect PAHs with the aid of practically designed substrates. Previously, single-strand DNA has been shown to electrostatically interact with the native oxide layer of aluminum through its phosphate backbone, enabling aluminum nanocrystal (AlNC) aggregates to be an effective SERS substrate for DNA detection. Herein we explore surface oxide engineering as a tool to promote stronger binding between the alumina shell of AlNCs and DNA. Annealing and washing in various environments (helium, vacuum, acid) can manipulate the surface chemistry of AlNCs to support unique interactions with analyte molecules. We aim to develop an AlNC aggregate-based substrate capable of detecting PAHs through the DNA-PAH adduct configuration.

G32 – High-density, large-scale recording and stimulating neural probes with integrated ASIC

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Ultraflexible nanoelectronic neural probes have shown their capabilities in stable long-term recording at a wide range of spatial-temporal scales and a high resolution from animal brains, thanks to their miniaturized electrode configurations and close-to-tissue mechanical compliance that contributes to a glial scar-free interface. These features also enable them to be integrated with imaging systems for neuron ensemble and vasculature study. However, current neural recording devices cannot record and process data from a large across-brain-region scale at a cellular level, while ensuring the free movement of the animal. Here, we present electron-beam lithography (EBL) fabricated high-density flexible probes with up to 512 channels. We revisit some design concerns as the dimensions of the interconnect wires shrink to a hundred-nanometer level, then describe the challenges of reaching a high fabrication channel yield and how we addressed them. Those probes record spikes from free-moving rats with little amplitude degradation over up to 3 months after implantation. We further propose an integration of ultraflexible polymer probes with a lightweight, densely packed application-specific integrated circuit (ASIC) that enables simultaneous thousand-channel recording with a headstage of minimal weight. This work will facilitate neuroscience studies in animal models, as well as clinical applications.

G33 – Shockwaves in Exponential Ultracold Neutral Plasmas

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Ultracold neutral plasmas (UNPs), formed by photoionizing a cloud of laser-cooled atoms, provide a powerful platform for studying various plasma phenomena due to experimental accessibility and precise control over initial conditions. They can be used to study a wide range of plasma physics, including hydrodynamic and kinetic phenomena, and magnetized and unmagnetized plasmas, as well as probe the impact of strong Coulomb coupling that is accessible because of the low temperature. The possible occurrence of shock waves in an UNP has been of interest since these systems were first created and their expansion was studied. In this talk, we will present evidence for shock waves in UNPs with an initial exponentially decaying density distribution. Signatures of shock waves exist in both the velocity and temperature profiles of the plasma.

G34 – Hubbard parameters for programmable tweezer arrays

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The experimental realization of Fermi-Hubbard tweezer arrays opens a new stage for engineering fermionic matter, where programmable lattice geometries and Hubbard model parameters are combined with single-site imaging. To use these versatile experimental Fermi-Hubbard models as quantum simulators, it is crucial to know the Hubbard parameters describing them. Here we develop methods to calculate the Hubbard model parameters of arbitrary two-dimensional lattice geometries: the tunneling t, on-site potential V, and interaction U, for multiple bands and for both fermions and bosons. We show several examples. One notable finding is that equally deep and separated tweezers give spatially non-uniform Hubbard parameters, and we demonstrate procedures to find trap configurations that equalize these parameters. More generally, these procedures solve the inverse problem of calculating Hubbard parameters: given desired Hubbard parameters, find trap configurations to realize them. These methods will be critical tools for using tunnel-coupled tweezer arrays. Our code is available on https://github.com/htwei17/HubbardTweezer.

G35 – Interplay between Cavity Quantum Electrodynamics and Superconductivity

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There is currently much interest in studying solids placed in optical cavities to uncover new phases and phenomena in the complete absence of any external fields other than the fluctuating vacuum, or zero-point, electromagnetic fields. Judicious engineering of the quantum vacuum surrounding the matter inside the cavity can lead to nonintuitive modifications of electronic states and novel properties. Here we study superconducting films inside terahertz cavities in search of some of the recently predicted phenomena such as enhancement of superconductivity via vacuum driving of quasiparticles or phonons as well as the formation of novel superconductor-cavity-polaritons. We measured the electrical resistivity – temperature relation of thin films of niobium nitride, a Bardeen-Cooper-Schrieffer-type superconductor, inside a cavity and compared with the free-space results. We also performed terahertz time-domain spectroscopy measurements to study the influence of cavity fields on the optical conductivity spectra of the films at various temperatures and magnetic fields. Preliminary results and future steps for uncovering new phenomena in the superconductor cavity light–matter coupled systems will be discussed.

G36 – Quasi-1D Spin-imbalance Fermi gas and a new Li quantum gas machine

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Quantum simulation of ultracold atomic Fermi gases provides an ideal platform to study the behavior of electrons in solid-state systems. One particular interest is the study of the finite momentum Cooper pair, also known as the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. The FFLO phase is believed to occupy larger phase space in low dimensions, whereas it is more robust against quantum and thermal fluctuations in high dimensions [1][2]. Therefore, our spin-polarized gas is prepared in the quasi-1d regime by tuning the inter-tube tunneling rate of a 2D optical lattice and the interaction strength via a magnetic Feshbach resonance. In this poster, we review our methods and progress toward the direct observation of the domain walls, where the periodicity of the domain walls is a consequence of an LO-type order parameters and finite momentum pairing.

We also present the design of a new all-optical Li Fermi gas machine as an upgraded workhorse for searching for the FFLO state with a higher image resolution and optical Fourier transformation to detect the periodic domain walls. Furthermore, we will implement Bragg spectroscopy to detect the paired and unpaired sound velocities as an additional probe for the FFLO-like phase [3]. This new apparatus also features a higher numerical aperture for our future 3D optical lattice experiment.

[1] M. M. Parish et al. Phys. Rev. Lett. 99, 250403 (2007)
[2] M. O. J. Heikkinen et al. Phys. Rev. B, 87, 224513 (2013)
[3] J.-F. Pan et al. Commun. Theor. Phys. 74, 125802 (2022)

G37 – Band Structure Evolution through Electron Doping in $CrGeTe_3$

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In condensed matter physics, van Hove singularities (VHSs) in the electronic structure of 2D materials produce a divergent density of states that is prone to electronic instabilities when tuned to the Fermi level, and therefore often associated with a precursor of new ordered phases. However, despite the previous fruitful studies on this topic, it is still challenging to understand the effects of VHSs and directly compare them to theoretical predictions, often due to a mixing of VHSs with other coexisting bands. Here, we have investigated a clean single-band system with isolated VHSs in a ferromagnetic semiconducting material $Cr_2Ge_2Te_6$ (CGT). By surface alkali metal doping, we were able to tune the VHS to near the Fermi level, hence creating a genuine 2D system suitable for investigating VHS-induced novel states and their interplay with magnetism. In this report, we will present our step-by-step *in situ* potassium doping experiments on pristine CGT crystals, tuning the Fermi level to go across the VHS level and beyond, while tracking the electronic band structure evolution through each step by implementing angle-resolved photoemission spectroscopy measurements. We identified a clear signature of band structure renormalization after the doping level passed the VHS, which could indicate an enhanced correlation in the partially filled conduction band. Additionally, we noticed that another set of shadow band appeared in the semiconductor band gap right under the conduction band bottom, shifting with electron doping, which could result from electrons coupling with bosonic modes in the system.

G38 – Chronic Characterization of Neuronal Network in Mouse Primary Somatosensory Cortex using Electrophysiology after Stroke

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Neural plasticity in response to trauma lies not only in the repair and regeneration of neuronal population, but also in the change of network topology. Recent advances in network neuroscience have facilitated analysis in stroke-induced connectivity change. Previous works have utilized imaging methods to characterize the slow-scale functional connectivity. However, their limits in temporal resolution restrict the quantification of fast spiking activity. Ultra-flexible neural electrodes enable us to study the change in connectivity pattern within a local neuronal population (i.e., transmission of action potentials) in the primary somatosensory cortex of mouse after stroke. Two primary questions guide our study: (A) are there chronic shifts in the laminar profile of electrophysiology? (B) other than characterizations in spatial domain, what changes in neuronal connectivity topology underlie the recovery process? To inspect the chronic differences in the laminar profile, we use *current source density* analysis, which reveals a slow shift of spatiotemporal response to sensory stimuli. To quantify connections between neurons, we employ *cross-correlogram* based approach and investigate in parallel both the faster-scale mono-synaptic connection and slower-scale synchrony in activation. Preliminary results suggest an intriguing increase in the ratio of long-vertical-distance excitatory connections; whereas the inhibitory connections tend to become more localized. The synchrony within the stroked primary somatosensory regions is disrupted and gradually recovers. Regarding topology beyond spatial domain, we observe increased network reachability post-stroke; eigenvector centrality analysis further suggests the occurrence of "hub" neurons may contribute to network recovery process.

UG01 – Electrochemical Determination of Total Arsenic Using Rodeostat

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Arsenic is a carcinogenic contaminant present in groundwater affecting millions of people worldwide. Arsenic pollution stems from natural and anthropogenic sources (e.g., mining and agriculture) and it is toxic in the low parts-per-billion (ppb) range. Arsenic quantitation remains challenging and/or costly for groups such as Caminos de Agua, a non-profit organization focused on ensuring arsenic-free water for disadvantaged communities in central Mexico. Currently, available arsenic quantitation methods have limited use in these contexts because of their cost and/or limited accuracy.

For this study, we collaborated with Caminos de Agua to improve and validate a system based on an open-source mid-range potentiostat (Rodeostat). Two groups, one at Rice and one at UTEP, built Rodeostat-based systems and tested arsenic solutions, spiked water, and arsenic-contaminated waters to compare their performance against state-of-the-art analytical methods performed by El Paso Water Utilities Water Quality Laboratory. Additionally, we edited and streamlined the user manuals for the Rodeostat.

Our results support the Rodeostat's potential for a more cost-effective, user-friendly, precise, and accurate detection tool for arsenic-contaminated waters in low-resource settings. Future work includes a more comprehensive evaluation of the Rodeostat system's precision and accuracy, redesigning the system to lower equipment costs, and streamlining the setup process for inexperienced users with the goal of producing a test kit that can be readily deployed and used extensively. Overall, this system illustrates the potential of mid-range potentiostats to provide an accessible and reliable arsenic measurement system for people and/or organizations without access to high-tech equipment.

UG02 – A New Mechanical Strain Device for ARPES

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Deformation in the nanoscale can alter a material's microscopic environment, which, in response, can potentially tune superconductivity and other exotic orders. To observe such tuning explicitly, one needs an in-situ strain device compatible with angle-resolved photoemission spectroscopy (ARPES), which can unveil the electronic structure evolution under the tuning of the emergent orders. However, the current state-of-the-art device is piezo-driven, which has a strict instrumentation requirement and is, therefore, hard to generalize and use. We aim to design new devices compatible with the home lab and most synchrotron facilities to resolve this issue. The devices are mechanically driven, hence do not require any built-in electrodes, and can generate controllable and repeatable strain states. Here, we present new types of screw-driven strain devices which couple the strain field to the real-space positions. The samples are attached to beams and undergo different uniaxial strain fields as the beams displace. The device geometry is designed to guarantee a wide strain distribution, allowing for five or more samples to be measured at once instead of just one sample, as in the piezo-driven device. The idea is firstly justified by Bernoulli-Euler beam theory which can characterize the displacement of the device's beams. Furthermore, we use the finite element methods in SOLIDWORKS and develop an algorithm that can extract the spatially dependent strain profile from the simulation results in an efficient manner. With this setup, we can improve the design and alter strain distributions until a desirable tool is created.

UG03 – Analysis of Implementation of Transformers and Convolutional Neural Networks for Accurate and Efficient RFFI Authentication

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In our research, we investigate Radio Frequency Fingerprint Identification (RFFI), a wireless device authentication method, more specifically its implementation using machine learning frameworks, which are trained to distinguish the identities of IOT devices by looking at their "fingerprint" - or minor distortions in the transmitted signal in its respective channel caused by imperfections in the manufacturing process of the device, giving each device its own "fingerprint". The main objectives of our research were to discover machine learning models which would train more quickly and more consistently classify device identities correctly. Starting with PyTorch first, we investigated how the Transformer model architecture, a popular natural language processing model, could serve us well, tweaking hyperparameters such as the number of encoder layers and learning rate used, keeping system overhead in mind. In an effort to reduce system overhead, we switched to convolutional neural network models designed to replace the Transformer model, trying both dynamic and lightweight convolutions. We moved forward with using our lightweight convolution model and tested permutations of different kernel sizes for 2 encoders, the number we found best, along with varying dropout rates for dropout layers that follow. We analyzed performance of the models by looking at their classification accuracy when given inputs of varying signal to noise ratio and all trained over the same number of epochs. We tried similar training methods in TensorFlow. Our goal is to implement the algorithms with the Vitis AI design tools to create an inference hardware accelerator for Xilinx FPGAs.

UG04 – A split and inducible adenine base editor for precise in vivo base editing

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DNA base editors use deaminases fused to a programmable DNA-binding protein for targeted nucleotide conversion. However, the most widely used TadA deaminases lack post-translational control in living cells. Here, we present a split adenine base editor (sABE) that utilizes chemically induced dimerization (CID) to control the catalytic activity of the deoxyadenosine deaminase TadA-8e. sABE shows high on-target editing activity comparable to the original ABE with TadA-8e (ABE8e) upon rapamycin induction while maintaining low background activity without induction. Importantly, sABE exhibits a narrower activity window on DNA and higher precision than ABE8e, with an improved single-to-double ratio of adenosine editing and reduced genomic and transcriptomic off-target effects. sABE can achieve gene knockout through multiplex splice donor disruption in human cells. Furthermore, when delivered via dual adeno-associated virus vectors, sABE can efficiently convert a single A•T base pair to a G•C base pair on the PCSK9 gene in mouse liver, demonstrating the first in vivo CID- controlled DNA base editing. Thus, sABE enables precise control of base editing, which will have broad implications for basic research and in vivo therapeutic applications.

UG05 – Low-Iridium Catalysts for Proton Exchange Membrane (PEM) Water Electrolysis

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As the energy sector transitions from fossil fuels to hydrogen for a clean fuel alternative in order to preserve our environment, research into green-hydrogen production has become of growing interest. Proton exchange membrane (PEM) electrolysis can be used to produce hydrogen, but its dependence on the scarce element iridium poses a challenge. Therefore, for this study, a minimal amount of iridium was determined to facilitate effective PEM electrolysis in conjunction with ruthenium. Research, configuration, and synthesis of ruthenium-iridium oxide at different ratios revealed a degree of stability/instability that could potentially be used in PEM electrolysis. The results indicate that the ratio of 90% ruthenium and 10% iridium were considered stable. By discovering and developing a new material for lower iridium loading for PEM electrolysis, we can uncover novel results that contribute to the metamorphosis of the energy sector and a cleaner environment.

UG06 – Grooming microstructures in a mouse model of a monogenic autism spectrum and neurodevelopmental disorder

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Cephalocaudal grooming among mice follows a fixed four-phase pattern. Aberrant self-grooming is a tool in translational research for assessing repetitive or patterned behaviors in autism spectrum and neurodevelopmental disorder (ASD/NDD).[1] This behavior is useful in understanding neural mechanisms of hierarchical motor control that underlie complex sequential behaviors in ASD/NDD.[2,3] We studied the grooming microstructure and motor stereotypies in a mouse model of a monogenic ASD/NDD due to *EBF3* loss of function gene changes affecting a protein critical for neurodevelopment.

Our grooming data was collected at 7 weeks and 24 weeks from a blinded cohort of mice in the open-source software BORIS. We recorded the duration of phases, phase transitions, and gaps in grooming. Grooming bouts containing the syntactic chain (1->2->3->4) were characterized as correct, and all other bouts were characterized as incorrect. General health assessments were obtained at weekly intervals for weight, kyphosis, tail lesions, hindlimb clasping, dystonia, and survival.

Grooming behavior analysis and general health assessment were conducted in the ASD/NDD mouse model. Increased duration of phases, within-phase transitions, and stereotypies among one genotype suggest the presence of repetitive behaviors in the mouse model. Additionally, assessment of phase transition frequency highlights the disruption of patterned behaviors and increased overall transitions, indicating a perturbation of grooming microstructure.

Although duration of grooming is a well-established technique to understand repetitive and stereotyped behaviors, our extensive analysis of grooming microstructure, transitions, and phase duration expands the utility of grooming behaviors in genetic mouse models of ASD/NDD.

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UG07 – Sustainable Water Treatment Proposal for a Small Periurban Community

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Globally, around 2 billion people lack access to safe drinking water, including in the United States, where marginalized communities, such as Hueco Tanks in El Paso County, lack basic drinking water and sanitation services. Like most colonias, Hueco Tanks is a rural, unincorporated, low-income, and predominantly Hispanic community, where many residents rely on “pipas" or water delivery trucks for showering and doing laundry. However, fears regarding the quality of the delivered water and their water storage tanks have led to financial and emotional strain for residents.

For this study, engineering and social work students from Rice and UTEP collaborated with the NGO Familias Triunfadoras to construct and present a sustainable and culturally-appropriate water treatment proposal to Hueco Tanks’ residents, who will be the final decision-makers. First, we divided the proposal into three points of intervention: the pipas, the storage, and the point-of-entry (POE) treatment, where each team conducted cost-benefit analyses and community surveys for each possible solution. Then, Hueco Tanks’ residents will be presented with the results and provide feedback to refine the solutions.

Our study supports that sustainable rural technology development requires a lifecycle design that involves the community right from the start to be successful. Future work includes reaching out to other NGOs working with colonias and continuing communication with Hueco Tanks residents. Overall, this proposal illustrates the potential of future solutions for other small rural communities in the U.S. that lack piped water and suffer from water scarcity.

UG08 – Are Your Hands on the Dash?: Evaluating Fairness of Florida's Traffic Stop Outcomes

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Over the past few years, there have been numerous policing incidents that have led people to wonder if there are demographic disparities in traffic stops. Even further, the use of predictive policing, which uses historical data and algorithms to identify potential criminal history, has become very popular. In light of this, we ask a series of questions: what information about the subject and the officer leads to certain outcomes? Using historical demographic traffic stop data, how accurately can we predict the outcome of a traffic stop? To answer these questions, we conduct a foundational analysis of Florida's statewide traffic stop data 2016-2018. We predict traffic stop outcomes and examine whether there are biases with respect to race and gender. Our work has implications for understanding bias and bias mitigation strategies in predictive policing.

UG09 – Monolithic Segmented Blade Ion Trap System

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Quadrupole-based traps are versatile tools for AMO research and specifically for the ion-trapping community widely used in quantum computing, simulation, and sensing. Despite the advances of planar chip microfabricated traps, three-dimensional blade traps still offer the advantages of ease of use (simpler controls), eV-deep trapping potentials, robustness to stray fields, larger ion-electrode distance (low heating rates), as well as wider and multi-directional optical access.

A monolithic segmented blade trap represents further advancement in the blade trap design as it offers better structural accuracy by eliminating the need for manual alignment, a compact structure, potentially more elaborate design, and better manufacturability and repeatability. Here we present our progress in assembling a compact trapping system based on a monolithic blade trap. We present the design of the trap manufactured by Translume Inc. and its characterization, as well as the surrounding vacuum and optical systems of the first prototype. Preliminary measurements show promising performance and support further development and implementation of this novel type of blade traps.

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UG10 – Complex magnetic order and magnetotransport in $EuAu_2Sn_2$ single crystals

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Rare earth intermetallics often display complex magnetic and transport properties, owing to the interplay between different energy scales such as Rudeman-Kittel-Kashuya-Yoshida (RKKY) interactions and crystal electric field effects (CEF). However, Europium ions have a half full 4f electronic shell, which means that the CEF should be absent in such compounds, and therefore the magnetic order is expected to be a simple collinear antiferro- or ferro-magnetic ground state. Our group has recently shown that a series or Eu-based intermetallics with square net crystal structure, Eu(Ga,Al)4, have complex magnetic and topological properties, even in the absence of CEF effects, prompting the need for finding the origin of the competing interactions other than CEF anisotropy. Through synthesis of high quality single crystals, I discovered that EuAu2Sn2 is a candidate magnetic topological system: temperature- and field-dependent magnetization and resistivity measurements reveal at least three magnetic phase transitions below 10 K, and relatively large magnetoresistance MR ~ 20% up to 9 T. I will discuss the detailed H-T phase diagram in this compound, and the possible origin of the anisotropy that leads to the apparent con-collinear magnetic order, responsible for the multiple magnetic transitions.

UG11 – Contactless Strain Detection with Michelson Interferometer

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Angle-resolved photoemission spectroscopy (ARPES) is a powerful experimental technique that can provide detailed information about the electronic band structure of a material. Recent efforts in the field of ARPES involve applying uniaxial strain fields to crystals as an effective way to tune the emergent order and band structure with devices driven by screws or piezo actuators, which are ultra-high vacuum compatible. However, the ultra-high vacuum requirement impedes the conventional measuring methods since it alters the attaching characterization of the uniaxial strain state of measured samples. To provide an insight of the strain, we are designing a contactless optical approach to accurately measure the length of the gap where the sample is glued on top of a piezo-driven device. We set up a Michelson Interferometer, which utilizes the interference pattern to monitor the change in the gap size. To validate the set up, we first realized an equivalent optical arrangement outside the vacuum environment. To support the measurement process, we developed a LABVIEW and MATLAB program, incorporating several key features:

- User-designed voltage profile
- Automatic recognition and annotation of anomalous data points
- Smart denoising
- Self-adjusted pattern recognition

UG12 – Water Insecurity in Hueco Tanks, El Paso County

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Access to clean and safe water is a basic human right. Yet, many marginalized communities, including colonias, unserved, or poorly served low-income housing settlements in the United States near the border along Mexico, face significant challenges in securing a reliable water source. Social work undergraduate students from the University of Texas at El Paso (UTEP) interviewed ten (N=10) families in the Hueco Tanks colonia in El Paso County to conduct a community assessment and learn about their water-related insecurity challenges. The assessment found that participants have lived in Hueco Tanks ranging from less than one year to more than 30 years, and all have been living without piped water in their homes since they moved in. Families in Hueco Tanks all have water delivered in a cistern truck referred to as 'la pipa,' whose water quality and source are unknown. However, residents reported that the water from the cistern trucks is not safe for human consumption, forcing them to buy bottled water, adding to their expenses. Residents use treatment methods such as chlorine tabs or liquid bleach to disinfect the water without proper technical knowledge resulting in under- or over-chlorination of the water. Consequently, one participant reported symptoms of eczema and other skin conditions. With these findings, we collaborated with a group of Rice and UTEP engineering undergraduate students to develop a proposal for a water purification system appropriate to the Hueco Tanks population's needs.

UG13 – Effect of Initial PFOA Concentration on Photocatalytic Oxidation Reaction Kinetics

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Perfluorooctanoic acid (PFOA) is a persistent organic pollutant widely used in various industrial and consumer applications. PFOA has been found in various water sources around the world, leading to significant environmental and health concerns due to its bioaccumulative nature. In recent years, photocatalytic oxidation has emerged as a promising approach for the remediation of PFOA-contaminated waters. However, studies exploring the effectiveness of the photocatalytic oxidation of PFOA often focus on concentrations not found in the environment (e.g., parts per million). As a result, the need for a rigorous study exploring the activity of different photocatalysts as a function of initial PFOA concentration is necessary. In this study, we investigated the effect of the initial PFOA concentration on the photocatalytic oxidation of PFOA over titanium dioxide (TiO_2) and boron nitride (BN) under ultraviolet light (UV-C, 254 nm). We observed that as the initial PFOA concentration decreased, the initial reaction rate of the oxidation reaction decreased as well over both TiO_2 and BN. The results of this study give insight (e.g., catalyst dosage, pH, reaction time, etc.) on how to optimize treatment processes targeting environmentally relevant levels of PFOA (i.e., ppb and ppt levels) using photocatalysis.

UG14 – High-level synthesis for computing spectrograms on FPGA in an RFFI system

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Radio frequency fingerprint identification (RFFI) is a process for classifying wireless devices by analyzing distortions in their signals caused by hardware imperfections. This analysis is performed using machine learning-based image processing techniques to classify the spectrograms of the devices. A signal's spectrogram is a two-dimensional visualization of how its spectrum of frequencies varies with respect to time. To mathematically calculate a spectrogram, the short-time Fourier transform (STFT) algorithm is used, which essentially divides the signal into sub-signals at different time intervals and takes the Fourier transform of each sub-signal, returning each Fourier transform as columns of a matrix. To efficiently calculate many spectrograms in an RFFI system, field-programable gate arrays (FPGA) can be used. FPGA are integrated circuits that are programmable after manufacturing, allowing them to be used for myriad purposes that require high computational efficiency or low power usage. To program FPGA, high-level synthesis (HLS) software can be used. HLS allows for the automated conversion of a program written in a programming language such as C or C++ to a register/transfer-level (RTL) design in hardware description language (HDL) such as Verilog or VHDL, which can in turn be used to program FPGA. HLS thus simplifies the process of FPGA programming by allowing programmers to use more familiar or intuitive programming languages for complex tasks. This research project explored the use of HLS to program an FGPA to compute spectrograms for pre-processing in an RFFI system.

UG15 – Design and validation of a 3D tissue engineered bone model to develop novel Ewing Sarcoma Therapeutics

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Ewing sarcoma (ES) is a pediatric cancer which affects bone and soft tissue. If the tumor metastasizes, survival rates can drop to 20%. Despite attempts to develop new therapies, survival rates have not improved for decades (Grohar, Pharm. Ther., 2013), as per lack of complete understanding of the cancer's pathology. Current models are typically in 2D, however they fail to showcase accurate, in-vivo-representative cellular responses to drug treatments and tumor cell mobility. Here, we present a 3D model made of collagen and hydroxyapatite (HA) to mimic the in-vivo environment of bone for encapsulation of ES cells to address current research approach inadequacies. Collagen gels with varying concentrations of collagen (5 or 10 mg/mL) and with or without HA addition were used. Collagen was neutralized and HA was added to the collagen before the solution polymerized. To test the gels' mechanical properties, compression testing was performed. Interestingly, we observed the hydrogel with the highest compressive strength was 5 mg/mL Col1 without HA (average compressive strength (CS) = 1661 Pa, coefficient of variation (CV) = 1.36). This compressive strength was non-significantly ($p > 0.05$, student's t test for all pairs) larger than other formulations. These findings were not consistent with our hypotheses and may be a result of sample preparation or mechanical testing discrepancies. In future studies we will compare morphology of cells cultured in hydrogels to patient samples. Creating a relevant 3D model will allow for more accurate investigations of ES which has clinical relevance in creating new treatments.

HS1 – Hierarchical porous PbO2/FTO electrode for electro-degradation of various emerging contaminants

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The non-active anode lead dioxide (PbO_2) is considered an excellent electrode for the degradation of pollutants in water, possessing favorable properties such as high electrical conductivity and cost-effective fabrication methods. While conventional flat film PbO_2 anodes have low surface area, hindering mass transfer and reducing the number of active sites, porous PbO_2 electrodes have emerged as an effective solution to improve their performance. Current studies focus on fabricating PbO_2 electrodes with only micron- or sub-micron-sized pores; however, in this project we explore an enhanced porous electrode encompassing pore sizes of both the nano and micron scale to further increase surface area and mitigate mass transfer limitations. Here, we present a hierarchical porous PbO_2 (HP-PbO_2)/ fluorine doped tin oxide (FTO) anode for electrodegradation of various prominent pollutants in water. Firstly, HP-PbO_2 electrodes were fabricated via polystyrene opal templating (using beads of 4 μm and 50 nm sizes) and electrochemical deposition. Upon template removal, our HP-PbO_2 electrodes exhibited a uniformly ordered, close-packed array of macropores (resulting from the removal of the 4 μm polystyrene spheres) along with mesopores (derived from the removal of the 50 nm polystyrene spheres within the larger cavities). The as-fabricated HP-PbO_2 electrode exhibited significantly enhanced electrocatalytic activity compared to both its macroporous PbO2 and film PbO2 counterparts, achieving an impressive 86.5% removal efficiency of sodium dodecyl sulfate (SDS) within a three-hour timeframe. Moreover, our hierarchical porous HP-PbO2 electrode also demonstrated excellent performance in degrading various other water contaminants, including diclofenac sodium salt (DSA) and rhodamine B dye.