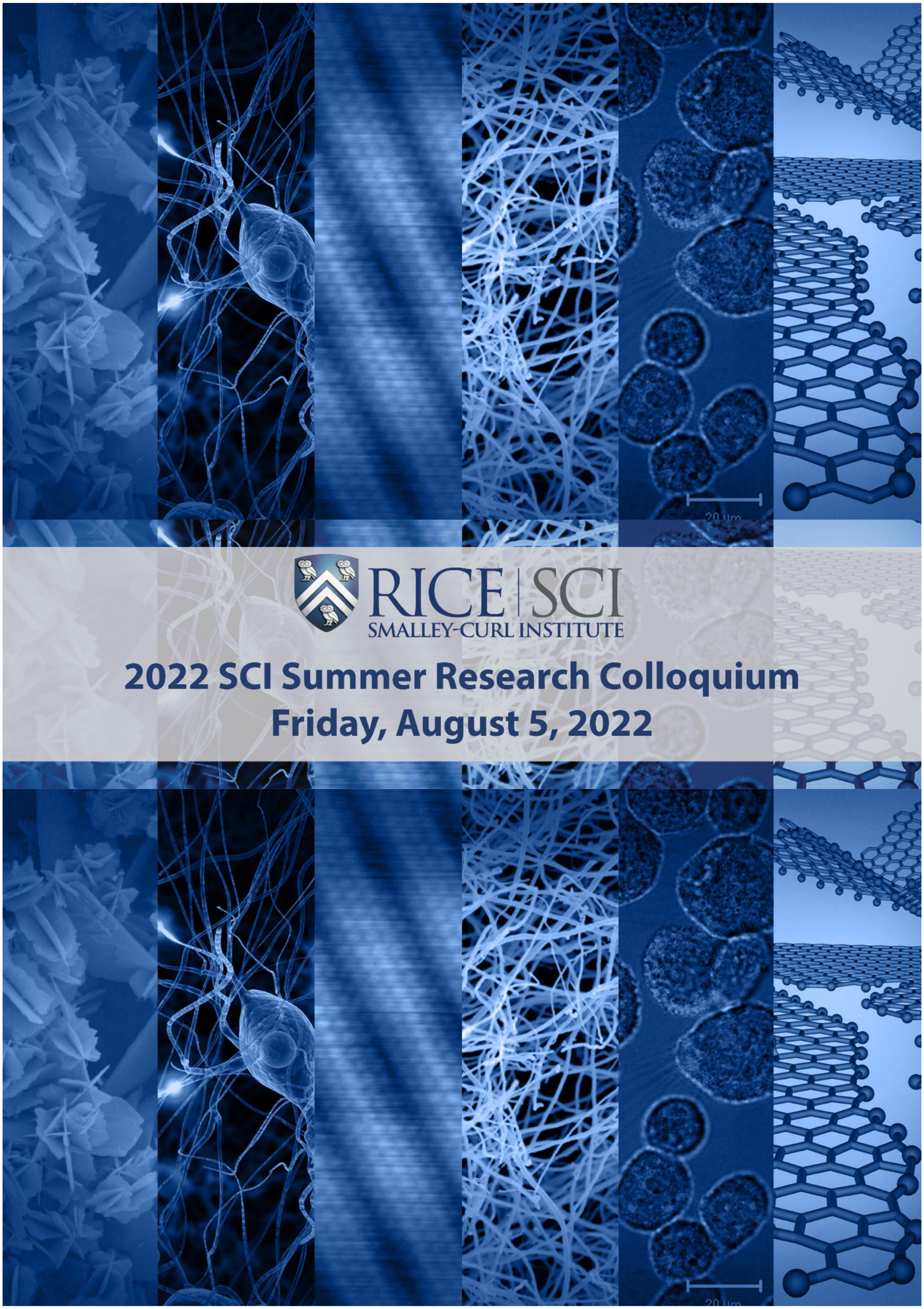

RICE | SCI
SMALLEY-CURL INSTITUTE

2022 SCI Summer Research Colloquium
Friday, August 5, 2022

2022 Smalley-Curl Summer Research Colloquium

Sponsors

LIGHT CONVERSION

MONTANA INSTRUMENTS®
COLD SCIENCE MADE SIMPLE

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

RICE UNIVERSITY
School of Engineering

RICE ENGINEERING
Electrical and
Computer Engineering

RICE | STEM
Office of STEM Engagement

Presentation Schedule

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

Oral session A (McMurtry Auditorium)

Session Chair: Manu Manjappa

9:00 am	**Gabriella Gagliano** “Single-objective tilted light sheet illumination with exchange-PAINT and Deep learning for fast, accurate, and precise 3D Super-resolution imaging in mammalian cells”
9:12 am	**Jiaming Luo** “Topological magnon-phonon hybridization in monolayer antiferromagnets”
9:24 am	**William Schmid** “Scalable solar thermal desalination: challenges and opportunities for light-to-heat conversion and energy recovery”
9:36 am	**Yigao Yuan** “Hydrogen generation with an earth-abundant plasmonic antenna-reactor photocatalyst and light-emitting diode-based illumination"
9:48 am	**Visal So** “Towards the analog quantum simulation of field theories with trapped ions”
10:00 am	**Weiyin Chen** “Flash recycling of Li-ion batteries”

Keynote

10:30 am	**Randy Hulet** “Quantum simulation with ultracold atoms”

Oral Session B (McMurtry Auditorium)

Session Chair: Gabi Gagliano

11:00 am	**Shengjie Yu** “Electronic transport in carbon nanotube fibers and bundles with ultrahigh conductivity”
11:12 am	**Tyler Nelson** “Construction and validation of a multimodal 3D Single-molecule super-resolution microscope for whole cell imaging”
11:24 am	**Minghe Lou** “Sustainable hydrogen production through plasmonic photocatalysis of Direct H_2S decomposition”
11:36 am	**Jaime Moya** “Signatures of real-space and reciprocal space Berry curvature by Hall measurements in the $Eu(Ga_{1-x}Al_x)_4$ system”
11:48 am	**Joshua Chen** “Self-rectifying magnetoelectric metamaterials enable remote neural stimulation and restoration of sensory motor functions”

12:00 pm **Lunch and Joint UG & Grad Poster Session** (Martel Hall)

(1:00 pm – 3:00 pm poster presentations)

Oral Session C (McMurtry Auditorium)

Session Chair: Adam Johnston

3:00 pm **Stephen Sanders** "Quantum enhanced sensing using lattice resonances supported by metallic nanohole arrays"

3:12 pm **Fuyang Tay** "Ultrastrong coupling in a three-dimensional photonic-crystal cavity"

3:24 pm **Mary Bajomo** "Computational chromatography: A machine learning strategy for demixing individual chemical components in complex mixtures"

3:36 pm **Dongyu Fan** "Structural heterogeneity and pH-dependent collapse behavior of weak polyelectrolyte brushes studied using 3D single molecule tracking"

3:48 pm **Tymofii Pieshkov** "Structure and composition of 2D interfaces"

4:00 pm **Han Yan** "Morse defects and fracton physics in spiral spin liquid and soft matter"

Oral Session D (McMurtry Auditorium)

Session Chair: Kunal Lakhanpal

4:30 pm **Diego Fallas Padilla** "Exploring classical chiral magnetism using a quantum Rabi ring"

4:42 pm **Elijah Kritzell** "Antiferromagnetic Resonance in NiO in Magnetic Fields up to 25 T"

4:54 pm **Kunhua Lei** "DNA Wrapping Causes strain in Single-Wall Carbon Nanotubes"

5:06 pm **Bryant Jerome** "Outcoupling Hyperbolic Modes from Aligned Carbon Nanotube Films"

5:18 pm **Angela Medvedeva** "Predicting antimicrobial activity for untested antimicrobial-peptide-based drugs in antibiotic resistant bacteria"

5:30 pm **Hao Zhang** "Direct visualization of ultrafast lattice ordering in 2D hybrid perovskites"

Award Ceremony and Dinner Cocktail (Martel Hall)

Keynote

Quantum Simulation with Ultracold Atoms

Randy Hulet

Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA

Strongly correlated electronic materials, a category that includes high-temperature superconductors and quantum magnets, have been at the focus of condensed matter physics for some time. These materials are extremely challenging to model with digital computers since the quantum vector space grows exponentially with the number of electrons. Furthermore, experiments with these materials are challenging to interpret due to the inevitable lattice defects, impurities, and the uncertainty of the screened Coulomb potential.

Quantum simulation may be realized with ultracold atoms replacing the electrons, and by engineering potential landscapes formed from the orderly interference of laser beams. These tools enable quantum simulation in a clean and highly tunable environment. I will describe how this works in two examples using ^{6}Li, a composite fermion: the undoped Hubbard model in three-dimensions (3D) [1]; and spin-charge separation of interacting fermions in 1D [2]. In both cases, we discovered unexpected new physics by comparing our measurements with advanced theory. To observe quantum magnetism in [1] required achieving temperatures as low as 1% of the Fermi temperature, a new record in 3D.

1. R. Hart, P.M. Duarte et al, *Nature* (2015).

Oral Presentations

<u>O-A-1</u> – Single-Objective Tilted Light Sheet Illumination with Exchange-PAINT and Deep Learning for Fast, Accurate, and Precise 3D Super-Resolution Imaging in Mammalian Cells

<u>Gabriella Gagliano</u>,[1,2,3] Nahima Saliba,[2] Dushyant Mehra[2], Anna-Karin Gustavsson[2,3,4,5,6]

[1]*Applied Physics Program, Rice University, Houston, TX, USA*
[2]*Department of Chemistry, Rice University, Houston, TX, USA*
[3]*Smalley-Curl Institute, Rice University, Houston, TX, USA*
[4]*Institute of Biosciences & Bioengineering, Rice University, Houston, TX, USA*
[5]*Department of Biosciences, Rice University, Houston, TX, USA*
[6]*Laboratory for Nanophotonics, Rice University, Houston, TX, USA*

Super-resolution fluorescence microscopy is a powerful method for imaging detailed biological structures at the nanoscale. However, the ability to image deep into samples such as mammalian cells is notoriously difficult due to increased fluorescence background in thick samples. One solution is light sheet fluorescence microscopy which uses a thin plane of light to optically section the sample, resulting in an increased signal-to-background ratio and thus an improved localization precision. In this work we present a single-objective tilted light sheet which we combine with four additional innovations: (i) a 3D-printed microfluidic chip, (ii) sequential DNA Point Accumulation for Imaging in Nanoscale Topography (DNA-PAINT) known as Exchange-PAINT, (iii) deep learning for improved localization precision and imaging speeds, and (iv) engineered point spread functions for 3D imaging. By combining light sheet illumination with Exchange-PAINT, we remove the need for low concentrations of imager strands and long imaging times, as background fluorescence from out-of-focus emitters is reduced. We further increase imaging speeds by combining Exchange-PAINT with deep learning to not only have control over the density of emitters but to reduce the requirement of sparse emitters by conventional analysis methods. In addition, sequential imaging using microfluidics allows for accurate multi-target imaging without chromatic aberrations. Taken together, our approach achieves improved localization precision, imaging speeds, and multi-target accuracy, enabling fast and precise multi-target 3D super-resolution imaging.

O-A-2 – Topological magnon-phonon hybridization in monolayer antiferromagnets

Jiaming Luo[1,4], Shuyi Li[2], Zhipeng Ye[3], Rui Xu[1], Han Yan[2], Junjie Zhang[1], Gaihua Ye[3], Lebing Chen[2], Ding Hu[2], Xiaokun Teng[2], William A. Smith[1], Boris. I. Yakobson[1], Pengcheng Dai[2], Andriy H. Nevidomskyy[2], Rui He[3], Hanyu Zhu[1]

[1]*Department of Materials Science and Nano Engineering, Rice University, Houston, TX 77005, USA*

[2]*Department of Physics and Astronomy, Rice University, Houston, TX 77005, U.S.A*

[3]*Department of Electrical and Computer Engineering, Texas Tech University, Lubbock, TX 79409, USA*

[4]*Applied Physics Graduate Program, Rice University, Houston, Texas 77005, U.S.A.*

Materials hosting topological bosonic excitations such as photons, phonons, and magnons potentially enable low-loss transport of information and energy in analogy to electronic topological materials. Compared with photons, phonons have smaller mode volume that can increase the coupling strength with spins to attain the quantum coherent regime and enable atomic-scale chiral topological bosons. Van der Waals (vdW) magnetic materials are promising to realize such states due to their recently discovered strong interactions among the electronic, spin, and lattice degrees of freedom. Here, we report the first observation of coherent topological hybridization of magnons and phonons in monolayer antiferromagnet FePSe3 by cavity-enhanced magneto-Raman spectroscopy. The robust magnon-phonon cooperativity in the 2D limit originates from the material's large single-ion anisotropy, weak interlayer exchange coupling, and bond-dependent spin-exchange interaction. We then identified nontrivial band inversion between longitudinal and transverse optical phonons caused by the strong coupling with magnons. The spin and lattice symmetry guarantees magnetic field-controlled topological phase transition that is also verified by first-principles calculations. The 2D topological magnon-phonon hybridization potentially offers a new route toward quantum phononics and magnonics with ultrasmall footprint.

O-A-3 – Scalable Solar Thermal Desalination: Challenges and Opportunities for Light-to-Heat Conversion and Energy Recovery

William Schmid,[1] Bryant Jerome,[1,2] Aleida Machorro,[1,2] Pratiksha D. Dongare,[1,3] Alberto Naldoni,[4] and Alessandro Alabastri[1,3]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[2]*Applied Physics Graduate Program, Rice University, Houston, TX, USA*
[3]*Laboratory for Nanophotonics, Rice University, Houston, TX, USA*
[4]*Department of Chemistry and NIS Centre, University of Turin, Turin, Italy*

In the search for effective technologies to relieve global water scarcity, thermal desalination has key advantages in terms of robustness and limited salinity dependence, making it a flexible choice for water treatment. Carrying electromagnetic energy, light can power thermal desalination if efficiently turned into heat. In the case of solar radiation, light-driven thermal desalination (LDTD) can lead to decentralized water purification, improving accessibility and reducing the environmental impact over conventional, heavy infrastructure-based desalination practices. However, there remains a lack of consensus on how to best design, evaluate, and compare the efficiency of diverse light-driven systems, particularly with respect to their day-long performance under natural, time-varying solar intensity. The scalability of evaporators, choice of materials, and the cost of other system components are also key elements for a comprehensive evaluation of a desalination system. We offer a blueprint for achieving efficient, scalable, and day-long LDTD. We argue that light energy is a means to an end for driving a thermal process in evaporation-based desalination systems. Critically, we discuss how minimizing environmental losses and maximizing heat recovery depend on each other, and their combination is paramount in bolstering the performance of real-world practical systems. By focusing on the optimization of system-wide thermal energy recovery and loss mitigation instead of the fabrication of advanced components only, and by exploiting dynamic energy recovery schemes that can be tuned adaptively for varying input power, highly efficient, cost-effective systems can be designed to take advantage of available light energy in the most general and flexible way.

O-A-4 – Hydrogen generation with an earth-abundant plasmonic antenna-reactor photocatalyst and light-emitting diode-based illumination

Yigao Yuan[1], Linan Zhou[2,4], Hossein Robatjazi[2,7], Junwei Lucas Bao[5,6], Jingyi Zhou[3], Aaron I. Bayles[1], Minghe Lou[1], Lin Yuan[1], Suman Khatiwada[7], Emily A. Carter[6], Peter Nordlander[2, 3], and Naomi J. Halas[1, 2, 3].

[1]*Department of Chemistry, Rice University, Houston, TX 77005, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX 77005, USA*
[3]*Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*
[4]*School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China,*
[5]*Department of Chemistry, Boston College, Chestnut Hill, MA 02467,*
[6]*Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, USA*
[7]*Syzygy Plasmonics Inc., Houston, TX 77054, USA*

Catalysts based on platinum group metals have been a major focus of the chemical industry for decades. Here we show that plasmonic photocatalysis can transform a thermally unreactive, earth-abundant transition metal into a catalytically active site under illumination. Fe active sites in a Cu-Fe antenna-reactor complex achieve efficiencies very similar to Ru for the photocatalytic decomposition of ammonia under ultrafast pulsed illumination. When illuminated with light-emitting diodes, the photocatalytic efficiencies remain comparable, even when the reaction scale is increased by nearly three orders of magnitude. This result demonstrates a highly efficient, electrically-driven production of green Hydrogen that can use earth-abundant species to drive this important chemical reaction.

<u>O-A-5</u> – Towards the analog quantum simulation of field theories with trapped ions

Visal So, Roman Zhuravel, Abhishek Menon, Midhuna Duraisamy Suganthi, and Guido Pagano[1]

Department of Physics and Astronomy, Rice University, Houston, Texas, USA

The high controllability, scalability, and long coherence times of trapped ions make them a promising platform for the analog simulation of many-body quantum spin systems. These features open up the possibility to study quantum field theories relevant for nuclear physics and high energy systems by mapping them to spin models with gauge invariant three-body or higher-order of interactions. Here, by extending and generalizing the Mølmer-Sørensen scheme, we propose to combine a single second-order spin-phonon excitation process with two first-order de-excitation processes. In this way, we can engineer an effective three-spin Hamiltonian beyond the traditional two-body interaction. Using this scheme, we propose an experimental setup to simulate the U(1) quantum link model, which approximates the lattice gauge field theory in 1+1 dimensions with trapped ions.

<u>O-A-6</u> – Flash Recycling of Li-ion Batteries

Weiyin Chen,[1] Rodrigo V. Salvatierra,[1] and James M. Tour[1,2,3,4]

[1]*Department of Chemistry, Rice University, Houston, TX, USA*
[2]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA*
[3]*Smalley-Curl Institute, Rice University, Houston, TX, USA*
[4]*NanoCarbon Center and the Welch Institute for Advanced Materials, Rice University, Houston, TX, USA*

The ever-increasing production of commercial lithium-ion batteries (LIBs) forebodes a staggering accumulation of waste when they reach their end of life. A closed-loop solution, with effective recycling of spent LIBs, will lessen both the environmental and economic cost of their use. Presently, <5% of spent LIBs are recycled and the regeneration of graphite anodes has unfortunately so far been mostly overlooked despite the considerable cost of battery-grade graphite. Here, we develop an ultrafast flash recycling method to regenerate the graphite anode and recover valuable battery metal resources. Selective Joule heating is applied within seconds to remove all resistive impurities with high energy efficiency. Subsequently, the as-formed inorganic salts, including lithium, cobalt, nickel, and manganese can be easily recollected using diluted acid (e.g., 0.1 M HCl), which cannot be achieved by directly leaching the black mass from the spent LIBs. As-prepared flash-recycled anode (FRA) preserves graphite structure, coated with a solid-electrolyte-interphase derived carbon shell, contributing to high initial specific capacity, superior rate performance and cycling stability, compared to anode materials recycled from high-temperature-calcination method. Life-cycle-analysis relative to current active materials production and recycling methods indicate that flash recycling can significantly reduce the total energy consumption and greenhouse gas emission while turning battery recycling into an economically advantageous process.

O-B-1 – Electronic Transport in Carbon Nanotube Fibers and Bundles with Ultrahigh Conductivity

Shengjie Yu,[1,2,3] Natsumi Komatsu,[1,3] Liyang Chen,[2,4] Renjie Luo,[4] Oliver S. Dewey,[3,6] Geoff Wehmeyer,[3,5] Matteo Pasquali,[3,6,7,8] Matthew Foster,[3,4] Douglas Natelson,[1,3,4] and Junichiro Kono[1,3,4,7]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[2]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, TX, USA*
[3]*Carbon Hub, Rice University, Houston, TX, USA*
[4]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[5]*Department of Mechanical Engineering, Rice University, Houston, TX, USA*
[6]*Department of Chemical Biomolecular Engineering, Rice University, Houston, TX, USA*
[7]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA*
[8]*Department of Chemistry, Rice University, Houston, TX, USA*

Macroscopic fibers of aligned carbon nanotubes (CNTs) with ultrahigh conductivity (> 10 MS/m) have recently become available, and they are expected to replace copper- or aluminum-based electrical cables in a variety of applications. For further conductivity improvement, a microscopic understanding of electronic transport processes in macroscopic CNT assemblies is required. For example, the roles of disorder, doping, and electron-electron interactions in determining the conductivity are not well understood. Here, we report results of our temperature- and magnetic field-dependent conductivity measurements on aligned CNT fibers and bundles produced by the solution spinning method. All samples showed a metallic behavior, i.e., conductivity monotonically increasing with decreasing temperature, in a wide temperature range from room temperature down to ~30 K. However, below 30 K, the conductivity decreased gradually with decreasing temperature. At low temperatures (<50 K), strongly temperature-dependent negative magnetoresistance appeared, which is a hallmark of weak localization, suggesting quantum coherent transport. In measurements on individual bundles exfoliated from a fiber, we observed fluctuations in conductivity as a function of magnetic field at low temperatures (<50 K), which can be interpreted universal conductance fluctuations.

<u>O-B-2</u> – Construction and Validation of a Multimodal 3D Single-Molecule Super-Resolution Microscope for Whole Cell Imaging

Tyler Nelson,[1,2] Sofía Vargas-Hernández,[1,3,4] Ivana Hsyung,[5] Margareth Freire,[6] and Anna-Karin Gustavsson[1,2,3,7]

[1]*Department of Chemistry, Rice University, Houston, TX, USA*
[2]*Smalley-Curl Institute, Rice University, Houston, TX, USA*
[3]*Institute of Biosciences and Bioengineering, Rice University, Houston, TX, USA*
[4]*Graduate Program in Systems, Synthetic, and Physical Biology, Rice University, Houston, TX, USA*
[5]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[6]*Department of Life Sciences, San Jacinto College, Houston, TX, USA*
[7]*Department of BioSciences, Rice University, Houston, TX, USA*

Single-molecule localization microscopy is a super-resolution technique which enables the investigation of structures and molecules in cells at a resolution surpassing the diffraction limit of light. The appropriate method with which to illuminate a sample varies according to the nature of the sample and the goals of the study, and there is typically a tradeoff between simplicity of use and optimal performance. Most commercial microscopes offer epi-illumination, where the entire sample is illuminated simultaneously. However, this creates high background fluorescence and increased risk of photodamage and photobleaching of the sample. Another commonly available illumination option is total internal reflection fluorescence (TIRF), where only a thin slice of the sample right at the coverslip is illuminated. This mode results in excellent contrast, but it is not compatible with whole-cell imaging. An alternative whole-cell compatible approach is light sheet illumination, where the sample is optically sectioned by a thin sheet of light introduced in a direction orthogonal to the detection axis.

In this work, we are building a flexible system using primarily commercially available parts which combines homogeneous flat-field epi- and TIRF illumination with the whole-cell sectioning capability of a light sheet. Our microscope will allow very fast switching between the illumination modes, all at several different laser wavelengths. In combination with a point spread function engineering system, our system will conveniently enable 3D super-resolution imaging and molecular counting in whole cells with an illumination mode that is optimized for the sample and region of interest.

O-B-3 – Sustainable Hydrogen Production through Plasmonic Photocatalysis of Direct H_2S Decomposition

Minghe Lou[1,4], Junwei Lucas Bao[3], Linan Zhou[1,4], Gopal Narmada Naidu[2,4], Hossein Robatjazi*[1,4,5], Henry O. Everitt*[2,4,6], Peter Nordlander*[2,4], Emily A. Carter*[3], and Naomi J. Halas*[1,2,4]

[1]Department of Chemistry, Rice University, Houston, Texas 77005, USA
[2]Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA
[3]Department of Mechanical and Aerospace Engineering and the Andlinger Center for Energy and the Environment, Princeton University, Princeton, New Jersey 08544, USA
[4]Laboratory of Nanophotonics, Rice University, Houston, Texas 77005, USA
[5]Syzygy Plasmonics Inc., Houston, Texas 77054, USA
[6]U.S. Army DEVCOM Army Research Laboratory, Houston, Texas 77005, USA

Plasmonic metal nanostructures have garnered rapidly increasing interest for their use as heterogeneous photocatalysts, facilitating chemical bond activation and overcoming the high energy demands of conventional fossil-fuel-based thermal catalysis. Here we introduce highly efficient, sustainable heterogeneous plasmonic photocatalysis of the direct decomposition of hydrogen sulfide into hydrogen and sulfur, an alternative to the industrial Claus process. Under visible-light illumination and with no external heat source, up to a 20-fold reactivity enhancement compared to thermal catalysis can be observed. We show that the substantially enhanced reactivity can be attributed to plasmon-mediated hot carriers that modify the reaction energetics. With a shift in the rate-determining step of the reaction, a new reaction pathway is made possible with a lower apparent reaction barrier. Light-driven one-step decomposition of hydrogen sulfide represents an exciting opportunity for high-efficiency hydrogen production and sulfur recovery at low temperatures, leading to a more sustainable petrochemical industry.

<u>O-B-4</u> – Signatures of real-space and reciprocal space Berry curvature by Hall measurements in the $Eu(Ga_{1-x}Al_x)_4$ system

Jaime M. Moya[1,2], S. Lei[2], K. Allen[2], Y. Gao[2], and E. Morosan[2]

[1]*Applied Physics Program, Rice University, Houston, TX, USA*
[2]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*

The origins of the Hall effect dates back to 1879 when Edwin Hall demonstrated that when a current flows through a conductor with an applied perpendicular magnetic field, a transverse voltage, now called the Hall voltage, appears from the charge carriers being deflected towards the edge of a material due to the Lorentz force of the magnetic field. Such Hall measurements are still used by engineers and scientists today determine the carrier type, concentration, and effective masses in conductive materials.

In the age of topological materials, it is now apparent that Hall effects can arise from an emergent property of materials called Berry curvature. This means a Hall effect can be generated without a magnetic field. In a material with a net non-zero Berry curvature, the Berry curvature acts as a source of magnetic flux and generates a Hall voltage. In condensed matter systems, Berry curvature can either be generated as a result of a material's topology in reciprocal space, or the topology of its spin texture in real-space. Here, I present Hall effect and thermodynamic measurements on a series of compounds belonging to the magnetic $Eu(Ga_{1-x}Al_x)_4$ family. In the magnetically ordered state, I find evidence of Berry-curvature resulting from what is constant with the real-space spin texture of a skyrmion – an exotic magnetic, particle-like spin texture with technological applications. In the field-polarized state, I find evidence for a giant anomalous Hall effect, likely a result of the topological band structure in reciprocal space.

<u>O-B-5</u> – Self-Rectifying Magnetoelectric Metamaterials Enable Remote Neural Stimulation and Restoration of Sensory Motor Functions

<u>Joshua C. Chen</u>,[1] Gauri Bhave[2], Fatima Alrashdan[2], Abdeali Dhuliyawalla[2], and Jacob T. Robinson[1,2]

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

Magnetoelectric materials can convert magnetic fields to electric fields and are used in applications ranging from wireless energy harvesting, sensing, to biotechnology. One such application that can take advantage of these materials is precisely timed wireless neural stimulation. While mm-sized magnetoelectric thin films have the necessary power densities to stimulate neural tissue, the kHz resonant frequencies at which these materials achieve those power levels are too high for excitable tissue to respond. Here, we demonstrate the first self-rectifying magnetoelectric metamaterial capable of modulating the high resonant frequency electric fields to low therapeutic frequencies, enabling wireless neuromodulation with high temporal resolution. This metamaterial uses nonlinear charge transport across nanometer semiconducting layers which allow the material to generate steady direct current voltages when powered by an alternating magnetic field. These magnetoelectric nonlinear metamaterials (MNMs) generate >1V biases and by pulsing the magnetic field at low frequencies, we can repeatably stimulate peripheral nerves with latencies of less than 5 ms. As a proof-of-principle, we demonstrate these MNMs to restore a sensory reflex in an anesthetized rat model as well as use the MNM to restore signal propagation in a severed nerve. Development of new metamaterials will enable future wireless bioelectronic implants spanning new applications such as magnetoluminescent materials to miniaturized electrochemical actuators.

O-C-1 – Quantum enhanced sensing using lattice resonances supported by metallic nanohole arrays

Stephen Sanders,[1] Mohammadjavad Dowran,[2] Umang Jain,[2] Tzu-Ming Lu,[3] Alberto M. Marino[2] and Alejandro Manjavacas.[4]

[1]*Department, Rice University, Houston, Texas, USA*
[2]*Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma, Norman, Oklamhoma, USA*
[3]*Center for Integrated Nanotechnologies, Sandia National Labratories, Albuqueqe, New Mexico, USA*
[4]*Instituto de Óptica (IO-CSIC), Consejo Superior de Investigaciones Científicas, Madrid, Spain*

Periodic arrays of nanoholes perforated in thin metallic films support lattice resonances that arise from the coherent multiple scattering enabled by their regular periodicity. These collective modes produce large electromagnetic near-field enhancements, which cause these systems to be very sensitive to changes in their dielectric environment. As a result, metallic nanohole arrays are an exceptional platform for the development of compact optical sensors that are capable of operating at the classical shot-noise limit. Therefore, in order to further improve their sensitivity, the sensor must be probed with quantum states of light, such as squeezed or entangled states. In this context, here, we provide a comprehensive analysis of the quantum enhanced sensing capabilities of metallic nanohole arrays with one and two holes per unit cell. We find that the two-hole array supports narrower and stronger lattice resonances compared with its one-hole counterpart, and therefore has a higher fundamental sensitivity limit, as defined by the quantum Cramér-Rao bound. Furthermore, we validate these findings with experimental measurements of the reflectance of representative sample arrays. The results of this work advance our understanding of the optical response of these systems and pave the way for developing optical sensors that are capable of taking full advantage of the additional resources offered by quantum states of light.

O-C-2 – Ultrastrong Coupling in a Three-Dimensional Photonic-Crystal Cavity

Fuyang Tay,[1,2,*] Ali Mojibpour,[1] Shuang Liang,[3,4] Andrey Baydin,[1,5] Arash Ahmadivand,[1] Nicolas Marquez Peraca,[6] Hongjing Xu,[6] Geoff C. Gardner,[4,7] Michael J. Manfra,[3,4,7,8,9] David Hagenmüller,[10] and Junichiro Kono[1,5,6,11]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX 77005, USA*
[2]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, TX, 77005, USA*
[3]*Department of Physics and Astronomy, Purdue University, West Lafayette, IN, 47907 USA.*
[4]*Birck Nanotechnology Center, Purdue University, West Lafayette, IN, 47907 USA.*
[5]*Smalley-Curl Institute, Rice University, Houston, TX, 77005, USA.*
[6]*Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA.*
[7]*Microsoft Quantum Purdue, Purdue University, West Lafayette, IN, 47907 USA.*
[8]*School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN, 47907 USA.*
[9]*School of Materials Engineering, Purdue University, West Lafayette, IN, 47907 USA.*
[10]*ISIS (UMR 7006), Université de Strasbourg and CNRS, 67000 Strasbourg, France.*
[11]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX 77005, USA.*

Recent developments in cavity quantum electrodynamics have demonstrated that the coupling of matter with vacuum fluctuation fields becomes nontrivial when the system enters a new regime called the ultrastrong coupling (USC) regime, paving the way for utilizing vacuum fluctuations to engineer quantum materials' properties and induce novel phase transitions. Many outstanding questions remain unanswered in such systems, including (i) whether multiple quasidegenerate photonic modes in a cavity can couple to each other through matter in the USC regime, collectively enhancing the light–matter coupling strength of the system, and (ii) how to design a cavity mode with a well-defined, finite in-plane wave vector that can couple to collective excitations in matter at large wave vectors. To address these questions, we have fabricated a three-dimensional photonic-crystal cavity (3D-PCC) with multiple cavity modes in a narrow frequency range and studied the coupling of the cavity modes to inter-Landau-level transitions. We used terahertz time-domain magnetospectroscopy to probe Landau polaritons with two orthogonal linear polarizations. The results confirm that our system is the first 3D-PCC system to reach the USC regime. The good agreement between experiment and theory indicates that there exists coupling between different cavity modes. The diffraction grating pattern of the 3D-PCC opens up the possibility of coupling the cavity modes with well-defined in-plane wave vectors to collective excitations below the light line. Our findings will enable further explorations of novel phenomena in the USC regime.

O-C-3 – Computational Chromatography: A Machine Learning Strategy for Demixing Individual Chemical Components in Complex Mixtures

Mary M. Bajomo[1,6], Yilong Ju[2], Jingyi Zhou[3,6], Simina Elefterescu[8], Corbin Farr[1,6], Yiping Zhao[9], Oara Neumann[5,6], Peter Nordlander[4,5,6], Ankit Patel[2,5,7]*, and Naomi J. Halas[1,4,5,6]*

[1]*Department of Chemistry, Rice University, Houston, Texas 77005, USA*
[2]*Department of Computer Science, Rice University, Houston, Texas 77005, USA*
[3]*Department of Materials Science and Nanoengineering, Rice University, Houston, Texas 77005, USA*
[4]*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*
[5]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA*
[6]*Laboratory for Nanophotonics, Rice University, Houston, Texas 77005, USA*
[7]*Department of Neuroscience, Baylor College of Medicine, Houston, Texas, 77030, USA*
[8]*Department of Biochemistry, University of Houston, Houston, Texas, 77204, USA*

Surface Enhanced Raman Spectroscopy (SERS) holds exceptional promise as a streamlined chemical detection strategy for biological and environmental contaminants compared to current laboratory methods. Priority pollutants such as polycyclic aromatic hydrocarbons (PAHs), detectable in water and soil worldwide and known to induce multiple adverse health effects upon human exposure, are typically found in multicomponent mixtures. By combining the molecular fingerprinting capabilities of SERS with the signal separation and detection capabilities of machine learning (ML), we examine whether individual PAHs can be identified through an analysis of the SERS spectra of multicomponent PAH mixtures. We have developed an unsupervised ML method we call Characteristic Peak Extraction (CaPE), a novel dimensionality reduction algorithm that extracts characteristic SERS peaks based on counts of detected peaks of the mixture. By analyzing the SERS spectra of two-component and four-component PAH mixtures where the concentration ratios of the various components vary, this algorithm is able to extract the spectra of each unknown component in the unknown mixture, which is then subsequently identified against a SERS spectral library of PAHs. Combining the molecular fingerprinting capabilities of SERS with the signal separation and detection capabilities of ML, this effort is a first step towards the computational demixing of unknown chemical components occurring in complex multicomponent mixtures.

O-C-4 – Structural heterogeneity and pH-dependent collapse behavior of weak polyelectrolyte brushes studied using 3D single molecule tracking

Dongyu Fan[1], Shahryar Ramezani Bajgiran[1], Farshad Safi Samghabadi [2], Chayan Dutta[3], Jacinta C. Conrad[2], Amanda B Marciel[1], Christy F. Landes[1,3, 4, 5]

[1]*Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[2]*Chemical and Biomolecular Engineering, University of Houston, Houston, TX, USA*
[3]*Chemistry, Rice University, Houston, TX, USA*
[4]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[5]*Smalley Curl Institute, Rice University, Houston, TX, USA*

Understanding molecular transport in polymer brushes is crucial for applications such as drug delivery, anti-fouling, and biosensors, where complex structural features of the polymer can control intermolecular interactions. Theoretical studies predict structural heterogeneity in polymer brushes, which is difficult to assess by conventional experimental methods. Here, we use a 3D single molecule tracking method based on phase engineering to quantify the motion of single probe molecules inside polymer brushes. This method can provide a nanoscale understanding of polymer brush properties and transport mechanism inside brushes. The additional complexity of the point spread functions (PSFs) in phase engineering methods requires parallel computing to improve the performance of an unbiased 3D tracking algorithm previously developed in our laboratory. We combine these experimental and computational methods to understand the interactions between a positively charged poly(*2*-(*N,N*-dimethylamino)ethyl acrylate) (PDMAEA) brush and an oppositely charged dye, Alexa Fluor 546. The probe transport behavior is monitored as the PDMAEA brush switches between collapsed and swollen states in response to pH change. Our results indicate different dominating factors (electrostatic forces vs steric effects) of intermolecular interactions at the nanoscale. Different transport components in the lateral and the axial direction suggest the physicochemical heterogeneity of the brush, providing microscopic insight into the dynamic change of polymer brush conformations.

O-C-5 – Structure and composition of 2D interfaces

Tymofii Pieshkov[1], *Jui-Han Fu*[2], *Lain-Jong Li*[3], *Yimo Han*[4]

[1]*Applied Physics Program, Rice University, Houston, Texas, USA*
[2]*Material Science and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia*
[3]*Mechanical Engineering, University of Hong Kong, Pokfulam, Hong Kong*
[4]*Materials Science and NanoEngineering, Rice University, Houston, Texas, United States*

In the world of 2D nanomaterials MoS_2 demonstrates outstanding electrical properties due to its ability to grow in monolayers on sapphire substrates. This creates opportunities for using it in future nanoelectronics. However, for maintaining high efficiency, the structure of MoS2 should have minimum number of misfits or inclusions of other elements. This indicates a need to understand the elemental composition of the 2D materials to atomic scales, and this is where techniques like scanning transmission electron microscopy (STEM)-energy-dispersive x-ray spectroscopy (EDX) come to aid. A key challenge in STEM-EDX is to increase the amount of signal from the sample without dealing too much damage to it by the electron beam. Thus here, we report a cross-correlation averaging method based on EDX datasets that can extract more useful information from the same datasets. EDX maps were acquired from a cross section sample of 2D monolayer MoS_2 grown on sapphire substrate. This method increases the signal-to-noise ratio of the elemental maps and diminishes the influence of sample or electron beam drift. Interestingly, the resulting line profile of the cross section provides evidence of the atomic composition of amorphous layer between the MoS_2 and the sapphire substrate. Based on our data, the amorphous layer has high amounts of Si in it along with sapphire elements – Al and O. Similar technique can be used for other 2D material cross section samples.

O-C-6 – Morse defects and fracton physics in spiral spin liquid and soft matter

Han Yan,[1] and Johannes Reuther[2]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[2]*Department of Physics, Free University Berlin, Berlin, Germany*

Spiral spin liquids are a class of spin liquids that feature a ring degeneracy of its ground states. Over the years, a concrete physical picture of its spin liquid nature has not been established, considering that its zero-temperature ground states do not admit any local degeneracy. In this work, we illustrate the low-energy structure of 2D spiral spin liquids and reveal its connection to fracton physics and cholesteric matter. We find that the local momentum vector can form new types of momentum vortices in the system, which have very different properties from the commonly known spin vortices [1]. Their proliferation leads the system into the spin liquid phase at low temperatures. Furthermore, the effective theory shows that these objects are equivalent to topological defects in the cholesteric matter, described by Morse theory with unusual fusion rules. Our work sheds light on the nature of classical spiral spin liquids and directly applies to the material $FeCl_3$ [2].

[1] H. Yan and J. Reuther, Low energy structure of spiral spin liquids, Phys. Rev. Research 4, 023175 (2022)
[2] Gao et al., Spiral spin-liquid on a honeycomb lattice, Phys. Rev. Lett. 128, 227201 (2022)

O-D-1 – Exploring classical chiral magnetism using a quantum Rabi ring

Diego Fallas Padilla,[1] Guo-Jing Cheng,[2] Yu-Yu Zhang,[2] and Han Pu[1]

[1]*Deparment of Physics and Astronomy, and Rice Center for Quantum Materials, Rice University, Houston, Texas 77251-1892, USA*

[2]*Chongqing Key Laboratory for strongly coupled Physics, Department of Physics, Chongqing University, Chongqing 401330, China*

Is not unusual that two seemingly very different systems are connected by the same underlying physics. Finding such connections can often help us to gain new insights into one system by importing knowledge obtained from the study of the other. Here we show how a light-matter interacting system, named the quantum Rabi ring, can be mapped to a magnetic system with various types of magnetic exchange couplings, allowing us to study ferromagnetic and antiferromagnetic ordering, as well as chiral magnetic structures, like skyrmions and magnetic vortices, in this quantum optics platform. We study how the geometry of the ring, namely, if the number of sites is odd or even, affects the phase diagram of the model. When the system has an odd number of sites, geometrical frustration stabilizes the chiral phases, a behavior previously reported in antiferromagnetic systems, allowing us to find an optical equivalent of the magnetic frustration phenomenon. This frustration not only generates a highly degenerate ground state but causes anomalous scaling exponents in the vicinity of the phase boundary. This work not only introduces a new candidate for simulation of few-body classical magnetic systems, but also emphasizes how we can use our accumulated knowledge of magnetic systems to explain features of systems that might not seem to be related to the former, at least at first glance.

<u>O-D-2</u> – Antiferromagnetic Resonance in NiO in Magnetic Fields up to 25 T

<u>Elijah Kritzell</u>,[1,2] Andrey Baydin,[1,3] Fuyang Tay,[1,2] Rodolfo Rodriguez,[4] Ikufumi Katayama,[5] Jun Takeda,[5] Hiroyuki Nojiri,[6] Henry O. Everitt,[1,7] Jing Shi,[4] Igor Barsukov,[4] and Junichiro Kono[1,3,8,9]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*
[2]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[3]*Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[4]*Physics and Astronomy, University of California, Riverside, Riverside, California, USA*
[5]*Department of Physics, Graduate School of Engineering Science, Yokohama National University, Yokohama, Japan*
[6]*Institute for Materials Research, Tohoku University, Sendai, Japan*
[7]*DEVCOM Army Research Laboratory-South, Houston, Texas, USA*
[8]*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[9]*Department of Material Science and NanoEngineering, Rice University, Houston, Texas, USA*

Antiferromagnetic materials have numerous advantages over ferromagnets such as characteristic frequencies in the terahertz range and the exhibition of ultrafast dynamics, and therefore are promising for information processing and spintronic devices. NiO has long been hailed as a prototypical example of an antiferromagnet. However, the complex magnetic properties of NiO have led to conflicting theoretical models. With the goal of more accurately and fully characterizing the resonances of NiO, we examine the magnetic field dependence up to 25 T using terahertz time-domain spectroscopy. Our results show both magnetic field dependent and magnetic field independent modes at about 1 THz. Furthermore, we utilize terahertz ellipsometry to examine the presence of additional modes below 1 THz. We synthesize these data sets to examine the efficacy of the conflicting sublattice models of NiO. Finally, we examine the rotational anisotropy and linewidth of the resonances.

<u>O-D-3</u> – DNA Wrapping Causes Strain in Single-Wall Carbon Nanotubes

<u>Kunhua Lei</u>,[1] Ali A. Alizadehmojarad,[1] Sergei M. Bachilo[1], and R. Bruce Weisman[1]

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

Short strands of single-stranded DNA (ssDNA) can disperse and individually suspend single-wall carbon nanotubes (SWCNTs) to form a class of hybrids with unusual properties and applications in nanotube structural sorting and fluorescence-based bioanalysis. In these hybrids, the ssDNA strands tend to physisorb onto the nanotube surface, coating it in helical or ring-shaped structures. We have carefully compared fluorescence spectral peak positions in samples of SWCNTs coated by ssDNA and in conventional surfactants such as SDS. In addition to the general and well-known spectral red-shift for the ssDNA-coated samples, we find a systematic dependence of both the E_{11} and E_{22} shifts on the *mod* 1 vs. *mod* 2 identity of the (*n*,*m*) species. This spectral pattern is characteristic of SWCNTs that are distorted by mechanical strain. We infer that the ssDNA wrapping exerts radial forces on the nanotube, causing this strain. The magnitude of the observed effect depends on the ssDNA oligo and on SWCNT diameter, with large values found for $(GT)_6$ and nanotubes with diameters near 0.9 nm. Atomistic molecular dynamics simulations show that $(GT)_6$ forms rings when coating such SWCNTs. Further insights into strain in ssDNA/SWCNT hybrids will be presented based on additional computations and experimental results.

O-D-4 – Outcoupling Hyperbolic Modes from Aligned Carbon Nanotube Films

Bryant Jerome, [1, 2] Ciril S. Prasad, [1, 2] Jacques Doumani, [1, 2] Oliver S. Dewey, [3] Andrey Baydin, [1, 4] Matteo Pasquali, [3, 4, 5, 6] Junichiro Kono, [1, 2, 4, 6, 7] Weilu Gao, [8] Alessandro Alabastri, [1, 4] and Gururaj V. Naik [1, 4]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX 77005, USA*
[2]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, TX 77005, USA*
[3]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX 77005, USA*
[4]*Smalley-Curl Institute, Rice University, Houston, TX 77005, USA*
[5]*Department of Chemistry, Rice University, Houston, TX 77005, USA*
[6]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX 77005, USA*
[7]*Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*
[8] *Department of Electrical and Computer Engineering, University of Utah, Salt Lake City, UT, USA*

Aligned carbon nanotube (CNT) films are hyperbolic metamaterials with abundant applications in a variety of fields, from optoelectronics to nanophotonics to thermal engineering [1]. Of particular interest is CNTs' ability to act as a thermal emitter within the mid-infrared [2]. Because of the extreme anisotropy of aligned CNT films, conductive along the alignment direction and dielectric in the other two, aligned CNT films possess hyperbolic dispersion [3]. Consequently, photons with very large momenta or high k-modes freely propagate within the aligned CNT material, making the medium interesting for a wide range of applications including engineering thermal emission. One of the challenges with hyperbolic materials is the extraction of high-k photons out of the medium. High k-modes within aligned CNT films do not outcouple to free space because of their extreme momenta. However, some of these high-k photons may be extracted out to the far-field via periodic gratings. Here, we demonstrate such outcoupling of high-k photons in aligned CNT films using 1D gratings. We optimize the grating design to observe enhanced absorption. This work demonstrates that aligned CNT films make an excellent hyperbolic material platform for infrared optics.

1. W. Gao, N. Komatsu, L. Taylor, G. V. Naik, K. Yanagi, M. Pasquali, and J. Kono, J. Phys. D 53, 063001 (2020).
2. W. Gao, C. F. Doiron, X. Li, J. Kono, and G. V. Naik, ACS Photon. 6, 1602–1609 (2019).
3. J. Elser, R.Wangberg, V.A. Podolskiy, and E. E. Narimanov, Appl. Phys. Lett. 89, 261102 (2006).

<u>O-D-5</u> – Predicting Antimicrobial Activity for Untested Antimicrobial-Peptide-Based Drugs in Antibiotic-Resistant Bacteria

Angela Medvedeva,[1,2] Hamid Teimouri,[1,2] and Anatoly Kolomeisky[1,2,3,4]

[1] *Department of Chemistry, Rice University, Houston, Texas, USA*
[2] *Center for Theoretical Biological Physics, Rice University, Houston, Texas, USA*
[3] *Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas, USA*
[4] *Department of Physics and Astronomy, Rice University, Houston, Texas, USA*

Antimicrobial peptides (AMPs) are peptides produced by eukaryotic and prokaryotic organisms, including humans, as the first line of defense against pathogens. Remarkably, a single AMP type that effectively halts bacterial growth can continue to exert significant antimicrobial activity when used in lower concentrations in combination with an ineffective AMP or resistant antibiotic, essentially sensitizing the bacteria to the antibiotic to which it was previously resistant. While decades of studies have tested AMP-AMP and AMP-antibiotic combinations against antibiotic-resistant bacteria, it is not feasible to test at the rapid rate needed all possible combinations against all possible bacteria. The process from drug production and discovery to testing and release into the market is resource-costly, which is why machine-learning methods including recommendation systems have been implemented to accelerate the identification of promising drug candidates. With machine-learning methods, existing data on AMP combination antimicrobial activity can be leveraged to narrow the pool of AMP combinations that need to be tested. The challenge is that when considering individual bacteria, the data on AMP and AMP-antibiotic, and AMP-AMP efficacy are sparse. In the current study, we applied multiple models that combat the sparsity problem to predict antimicrobial activity of individual AMP types and AMP-AMP and AMP-AB combinations. With high predictive model accuracy, we identified potential candidates with predicted antimicrobial activity for various antibiotic-resistant bacteria that can be experimentally tested for comparison against our predictions.

O-D-6 – Direct visualization of ultrafast lattice ordering in 2D hybrid perovskites

Hao Zhang[1,2], Wenbin Li[1,2], Joseph Essman[1], Claudio Quarti[3,4], Isaac Metcalf[5], Wei-Yi Chiang[6], Siraj Sidhik[1,5], Jin Hou[5], Austin Fehr[1], Stephan Link[6,7], Xijie Wang[8], Uwe Bergmann[9,10], Mercouri Kanatzidis[11], Claudine Katan[3], Jacky Even[12], Jean-Christophe Blancon[1] and Aditya Mohite[1,5]

[1]Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA
[2]Applied Physics Program, Smalley-Curl Institute, Rice University, Houston, TX, USA
[3]Univ Rennes, ENSCR, INSA Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, Rennes, France
[4]Laboratory for Chemistry of Novel Materials, Department of Chemistry, University of Mons, Place du Parc 20, Mons, Belgium
[5]Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA
[6]Department of Chemistry, Rice University, Houston, TX, USA
[7]Department of Electrical & Computer Engineering, Rice University, Houston, TX, USA
[8]SLAC National Accelerator Laboratory, Menlo Park, CA, USA
[9]PULSE Institute, SLAC National Accelerator Laboratory, Stanford University, Stanford, CA, USA
[10]Department of Physics, University of Wisconsin–Madison, Madison, WI, USA
[11]Department of Chemistry, Northwestern University, Evanston, Illinois, USA
[12]Univ Rennes, CNRS, Institut FOTON (Fonctions Optiques pour les Technologies de l'Information), UMR 6082, CNRS, INSA de Rennes, Rennes, France.

Direct visualization of ultrafast coupling between charge carriers and lattice degrees of freedom in photo-excited semiconductors has remained a long-standing challenge and is critical for understanding the light-induced physical behavior of materials under extreme non-equilibrium conditions. Here, by monitoring the evolution of the wave-vector resolved ultrafast electron diffraction intensity following above-bandgap high-density photo-excitation, we obtain a direct visual of the structural dynamics in monocrystalline 2D perovskites. Analysis reveals a surprising, light-induced ultrafast lattice ordering resulting from a strong interaction between hot-carriers and the perovskite lattice, which induces an in-plane octahedra rotation, towards a more symmetric phase. Correlated ultrafast spectroscopy performed at the same carrier density as ultrafast electron diffraction reveals that the creation of a hot and dense electron-hole plasma triggers lattice ordering at short timescales by modulating the crystal cohesive energy. Finally, we show that the interaction between the carrier gas and the lattice can be altered by tailoring the rigidity of the 2D perovskite by choosing the appropriate organic spacer layer.

Poster presentations: graduate students and postdocs

GP-1 – Ultra-high loading of coal-derived flash graphene additives in epoxy composites

Paul A. Advincula,[1] Wei Meng,[2] Lucas J. Eddy,[1,3] Jacob L. Beckham,[1] Duy X. Luong,[1,4] Satish Nagarajaiah,[2,5] and James M. Tour[1,3,6,7]

[1]*Department of Chemistry, Rice University, Houston, TX, USA*
[2]*Department of Civil and Environmental Engineering, Rice University, Houston, TX, USA*
[3]*Smalley-Curl Institute for Nanoscale Science and Technology, Rice University, Houston, TX, USA*
[4]*Applied Physics Program, Smalley-Curl Institute, Rice University, Houston, TX, USA*
[5]*Department of Mechanical Engineering, Rice University, Houston, TX, USA*
[6]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA*
[7]*Welch Institute for Advanced Materials, Rice University, Houston, TX, USA*

Graphene has been shown to be an exceptional reinforcing additive for composites, but the high cost of graphene synthesis has largely prevented its use on industrial scales. Flash Joule heating (FJH) provides a rapid, bulk-scale method for graphene synthesis from coal materials such as metallurgical coke (MC) into flash graphene (MCFG), allowing for preparation of composites with much higher proportions of graphene than have previously been achieved in the literature. Here, we investigate the properties of graphene-epoxy composites in a high nanofiller content regime. Composites with 20-50 wt% loading of MCFG were prepared by dispersing MCFG in a solution of diglycidyl ether bisphenol A epoxy precursor (DGEBA) and 1,5-diamino-2-methylpentane through magnetic stirring and high-shear mixing, followed by curing. These MCFG:DGEBA composites exhibit greatly increased elastic modulus, hardness, compressive strength, maximum strain and toughness. With a 1:4 ratio of MCFG:DGEBA, the Young's modulus and hardness of the epoxy are increased by 56% and 49%, respectively. Additionally, compressive strength is increased by 145% and the maximum strain is increased by 61% in the 1:4 ratio of MCFG:DGEBA. Furthermore, the toughness of the composites is optimized at a ratio of 1:3 MCFG:DGEBA with an increase of 496%. These results demonstrate that MCFG can be used both as a reinforcing additive and filler in epoxy composites. As the cost of FG plummets, since it can be produced from very low cost materials like MC, in milliseconds with no solvent or water, the prospects are promising for its high-loading use in composites.

GP-2 – Enhancement of Guanine Functionalization of SWCNTs with Metalloporphyrins

Ali A. Alizadehmojarad[1], Sergei M. Bachilo [1], and R. Bruce Weisman[1]

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

Single-wall carbon nanotubes (SWCNTs) have attracted tremendous attention because of the wide variety of their structure dependent electronic characteristics. Semiconducting SWCNT band gaps can be engineered with chemical modification of SWCNT side walls using reactive functional groups. Our lab recently discovered that guanine nucleobases of single-stranded DNA wrapping around the SWCNTs can chemically attach to their side wall in the presence of singlet oxygen. Here, we examined the kinetics of the guanine functionalization of SWCNTs with singlet oxygen generated via UV irradiation of metalloporphyrins. We additionally probed the guanine functionalization of (6,5) SWCNTs via singlet oxygen directly generated using visible and near-infrared irradiations, whose wavelengths respectively match the (6,5) SWCNT E_{22} and E_{11} exciton resonance. We found that the quantum efficiency of guanine functionalization with photosensitizer dyes is significantly greater than with direct singlet oxygen generation.

GP-3 – Elucidating the role of the amphiphilic ligand shell on the Au_{32} nanocluster

Arzeena S. Ali,[1] Fatima Akilo,[1] and Matthew R. Jones[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas 77005, USA*
[2]*Department of Materials Science & Nanoengineering, Rice University, Houston, Texas 77005, USA*

Nanoparticle synthesis is a well-developed field, but there are many questions about synthesis mechanisms. A common synthetic approach is the seed-mediated method, where small nanoparticle precursors are added to a growth solution to induce heterogeneous nucleation, yielding well-defined nanocrystals. Although the method is ubiquitous and simple, the size, shape, and chemical properties of the seeds remain poorly understood, limiting our understanding of further growth mechanisms. Recently, we discovered that a major component of the seed solution utilized for seed-mediated synthesis is an atomically precise gold nanocluster capped by amphiphilic alkyl quaternary ammonium ligands: $Au_{32}X_8[AQA^+{\bullet}X^-]_{12}$ (X = Cl, Br; AQA = alkyl quaternary ammonium). The presence of amphiphilic ligands implies the possibility of a bilayer structure, consisting of distinct inner and outer leaflets that stabilize Au_{32} and allow for ligand exchange. The stability and dynamics of the bilayer will dictate its ability to act as a nucleation site for particle growth. Here, we developed a mathematical model to predict outer leaflet AQAX properties based on the molecular packing parameters originally described by Israelachvili for amphiphile self-assembly. Cyanide-mediated etching results corroborate the model by confirming dialkyl dimethylammonium ligands (double tail, DT) reside more favorably within the outer leaflet than AQA ligands (single tail, ST), prolonging the stability of Au_{32} through a less dynamic outer leaflet. Mass spectrometry indicates that increasing lengths of DT ligands have a decreasing preference for residing within the inner leaflet. These results demonstrate that the strongly bound outer leaflet ligands have implications for mechanisms of cluster growth.

GP-4 – Engineering the Surface Chemistry of Aluminum Nanocrystals

Aaron Bayles[1,5], Lin Yuan[1,5], Adebola Ogundare[1,5], Minghe Lou[1,5], David Solti[1,5], Parmeet Dhindsa[1,5], Corbin Farr[1,5], Benjamin D. Clark[1,5], Yelsin Mendez[3], Henry Everitt[6], Peter Nordlander[4,5], and Naomi Halas[1,2,4,5]

[1]Department of Chemistry, Rice University, Houston, Texas 77005, USA
[2]Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA
[3]Department of Materials Science and NanoEngineering, Rice University, Houston, Texas 77005, USA
[4]Department of Physics &Astronomy, Rice University, Houston, Texas 77005, USA
[5]Laboratory for Nanophotonics, Rice University, Houston, Texas 77005, USA
[6]U.S. Army DEVCOM Army Research Laboratory - South, Houston, Texas,77005, USA

Aluminum nanocrystals (Al NCs) are a potentially more sustainable, earth-abundant alternative to Au and Ag for plasmonics applications. While the synthesis of Al nanocrystals of various shapes and sizes with a range of insulating and semiconducting coatings has been demonstrated by our group, the thin aluminum oxide layer that grows on the surface of these particles following their synthesis has never been fully characterized or controlled. Here we introduce the use of various annealing strategies to manipulate the electronic and chemical properties of the native oxide surface layer of Al NCs as a means to modify surface morphology and catalytic reactivity. The native oxide is an amalgam of amorphous alumina consisting of tetrahedral, octahedral, and defect sites. High-temperature annealing in an oxygen atmosphere crystallizes the oxide, enhancing stability, while annealing under vacuum induces higher defect densities on the nanocrystal surface, increasing catalytic reactivity. Solid-state NMR is used to quantify the various alumina coordination sites for each sample, which in turn correlates to modifications in catalytic activity for the NH_3 and MeOH decomposition reactions.

GP-5 – Trajectory classification via machine learning

Jagriti Chatterjee,[1] Chayan Dutta,[1], and Christy F. landes[1,2]

[1]Department of Chemistry, Rice University, Houston, Texas 77005, USA
[2] Smalley-Curl Institute, Rice University, Houston, Texas 77005, USA

Understanding transport processes in complex environments such as inside the biological cells or inside porous polymers is challenging. Often, such complex transport processes involve confined diffusion due to physical constriction of particles or directed motion due to external factors such as ATP-dependent transport through microtubules. Single particle tracking measurements with sub-10 nm spatial resolution and sub-100 ms time resolution is capable of measuring such complex dynamics whereas state-of-the-art particle tracking algorithms can identify particle positions to provide single-particle trajectories. Generally, such trajectories can consist of different types of particle motion such as Brownian diffusion, confined diffusion and directed transport. Analysis of the underlying physical motion is challenging for complex motion specifically multiple types of diffusion modes within one single trajectory can complicate data analysis with single mean-square analysis. Here, we developed a classification algorithm based on random forest architecture. We simulated 5000 trajectories for each motion type using Monte Carlo approach and trained the models with 6 features. The trained model was evaluated by the out-of-bag (OOB) data and accuracy was calculated to define the efficiency of the model. The balanced accuracy was found to be 78.44% with an average error rate for all motion types as 21.56%. Finally, the developed random forest model was applied to experimental trajectories with mixed motion, which helps in successful characterization of each sub-trajectory by its basic motion type features.

GP-6 – Automated Image Analysis for In-Situ Observation of MoS_2 grown on Chemical Vapor Deposition (CVD)

Faizal Arifurrahman[1], Tianshu Zhai[1], Jing Zhang[1], Andrew Hitt[1], Ming Tang[1], Jun Lou[1]

[1]*Department of Materials Science and Nanoengineering, Rice University, Houston, Texas, USA*

Two-dimensional (2D) Transition metal dichalcogenide (TMD) materials have attracted extensive attention because of their exotic properties for various advanced applications. Scalable and high-quality 2D TMD materials can be obtained by characterizing their morphology. The morphology encodes a wealth of information about the kinetic and structural properties of the materials, the growth process, and their environmental influence. The direct in situ observation is seen to play a crucial role in establishing the understanding of the growth mechanism and controlling the morphology of 2D TMD materials. Eventhough, it remains limited due to the difficulty of obtaining high-resolution images at high temperatures while maintaining the evolution of 2D TMD materials.

Our study of MoS_2 chemical vapor deposition (CVD) grown using an optical microscope indicates that the Mo:S ratio, chamber total pressure, and temperature produce diverse crystalline morphologies. Here, image pre-processing that enhances the image quality is combined with an object detection algorithm. By using this computer vision technique, we can track every individual crystal and its cluster formed by the coalescence of crystal with adjacent neighbors in steps.

GP-7 – Aluminum {111} Nanocrystals: Mechanisms Behind the Morphology

Parmeet K. Dhindsa,*[,1,3] David Solti, *[,1,3] Christian R. Jacobson, *[,1,3] Anvy Kuriakose,[2,3] G. Narmada Naidu,[2,3] Aaron Bayles,[1,3] Yigao Yuan,[1,3] Peter Nordlander,[2,3] and Naomi J. Halas,[1,2,3]

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

Metallic nanocrystals (NCs) with localized surface plasmon resonances (LSPRs) have received enormous interest due to their strong optical response generating many applications such as plasmonic photocatalysis, enhanced sensing, photothermal heating, and environmental remediation. Al NCs with well-defined size and shape are a promising earth-abundant supplement to traditional noble metals Au and Ag for plasmonic applications. Recent developments in Al NCs synthesis have shown that shape control of Al NCs is achievable using transition-metal catalyst for decomposition of Al precursor. However, the explicit role played by the catalyst in shape direction is not fully understood. Here, we demonstrate functional variants of titanocene dichloride (Cp_2TiCl_2) as effective catalysts for a simple one-pot colloidal synthesis of size-tunable {111}-faceted single-crystalline Al octahedra and single-twinned trigonal prisms by AlH_3 catalyzed decomposition. We further our understanding of Al-shape control kinetics through spectroscopic studies of the surface of our nanocrystals, demonstrating that molecular titanocene species act as capping agent and directs the final morphology. When the effective concentration of catalyst on the Al surface falls below a critical value during growth, the seeds evolve from pure{100} morphologies to pure {111} morphologies. Finally, the optical properties of {111}-faceted Al NCs are probed using single-particle darkfield spectroscopy. This work enables us to understand the catalyst role in Al shape growth. Modification of the molecular structure of the catalysts would potentially allow us to expand available Al FCC nanostructures, broadening the scope of Al for plasmonic and nanophotonic applications.

*These authors contributed equally.

GP-8 – Towards a light-shift gate with transverse momentum transfer from spatially modulated light

Midhuna Duraisamy Suganthi,[1] Visal So,[2] Abhishek Menon,[2] Roman Zhuravel,[2] and Guido Pagano[2]

[1]*Applied physics, Rice University, Houston, Texas, United States*
[2]*Physics and astronomy, Rice University, Houston, Texas, United States*

Ions trapped in a chain act as effective two-level systems that can interact with one another using gate operations and can be used to simulate spin quantum systems. Recently, a light shift gate has been demonstrated using the quadrupole transition in $^{171}Yb^{+}$ ions [1]. It offers advantages over the Molmer-Sorensen gate as it is insensitive to optical phases and is based on axial normal modes excitations that are more evenly spaced and reduce crosstalk. However, the gate is still sensitive to motional phase and that requires that the ions be placed at even-integer multiples of $\pi/\Delta k$. This becomes a constraint for long ion chains. We plan to use an array of individual beams orthogonal to the trap axis, where each beam has a gradient in its transverse spatial profile that can excite the axial modes of motion [2] [3]. We propose to use a spatial light modulator as the beam shaping tool for momentum transfer from the beam and also gain freedom in beam positioning. We illustrate how to realize a light-shift gate using this setup and discuss methods to generate the desired beam shape using the spatial light modulator.

[1] C. H. Baldwin, B. J. Bjork, M. Foss-Feig, J. P. Gaebler, D. Hayes, M. G. Kokish, C. Langer, J. A. Sedlacek, D. Stack and G. Vittorini, *Phys. Rev. A,* vol. 103, no. 1, p. 012603, 2021.

[2] A. D. West, R. Putnam, C. W. C. and P. Hamilton, *Quantum Science and Technology,* vol. 6, p. 024003, 2021.

[3] Felix Stopp, Maurizio Verde, Milton Katz, Martin Drechsler, Christian T. Schmiegelow, Ferdinand Schmidt-Kaler, *Arxiv:*2206.04894, 2022.

GP-9 – Conjugated porous organic polymers for tunable acid sensing

Jessica Gayle,[1] Soumyabrata Roy,[1] Kristen Miller, [1] Galio Guo,[1] Sakib Hassan,[2] Adwitiya Rao,[3] Chandra Singh[3] Jacob Robinson,[2] and Pulickel Ajayan[1]

[1]*Material Science and Nanoengineering, Rice University, Houston, Texas, U.S.A.*
[2] *Electrical and Computer Engineering, Rice University, Houston, Texas, U.S.A*
[3] *Department of Material Science and Engineering, University of Toronto, Ontario, Canada*

Conjugated porous organic polymers (POPs) offer unique properties that can support the rapid, sensitive, reversible, and robust sensing of volatile analytes. Theses rigid carbon bonded structures can often possess offer high thermal and chemical stability in harsh environments. The high conjugation and tailorable functionalities within these materials provide great potential of using these materials for tunable, reversible, and robust, colorimetric sensors. The addition of microporosity and high surface areas within these materials provides better access to gas species for improved detection and sensitivity. Although POPs show great potential for detection of volatile gas, the high aromaticity and conjugation within these structures often leaves these materials in an insoluble powder that is difficult to process into workable films for devices. In this study, four highly conjugated POPs with different conjugation and nitrogen moieties are studied for colorimetric detection of hydrogen chloride (HCL). All films were easily fabricated into films using a rapid and scalable drop cast approach. Films are composed of few nanometers layered sheets and possess thermal and chemical stability in common organic solvents. All films were sensitive enough to detect HCL gas down to 0.05ppm, far exceeding the required permissible exposure limit. The incorporation of tertiary nitrogen within TZ-TP and TAPA-TP structures lead to higher sensitivity during short exposure times and larger observable color change during longer exposure times, respectively. These films were then incorporated into an optoelectronic device that showed higher sensitivity and good recyclability of these films for real-time sensing.

GP-10 – X-ray diffraction study of supramolecularly assembled gold nanowires

Theodor Gerrard-Anderson,[1] David Marolf,[1] and Matthew Jones[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas, USA*
[2]*Department of Materials Sciences and Nanoengineering, Rice University, Houston, Texas, United States*

Gold nanowires have garnered interest in recent years owing to simultaneously being highly conductive and highly flexible, as well as having an extremely high surface area to volume ratio which causes surface chemistry to highly affect their physical properties. These attributes make them a promising material for the fabrication of thin transparent electronics, nanoscale circuitry, and mechanical and chemical sensing applications. Most attempts to fabricate nanowires into devices involving the use of drying force and sheer alignment effects to create large thin films; however, these techniques lack the control over nanowire position and orientation within the assembly that is required for more complex device fabrication. In this work we have developed a method to functionalize the surface of ultrathin gold nanowires with ligands whose supramolecular chemistry is strongly responsive to environmental stimuli such as temperature, pH, cation valency, and ionic strength of the solution. This functionalization involves a phase transfer from hexane (the solvent of the crude nanowires) to water, a solvent which is ideal for these supramolecular interactions. Phase transfer of these nanowires is a process which has been difficult to achieve in the field so far and unlocks this suite of supramolecular interactions which can be used to direct the nanowire assembly. Recent X-ray diffraction data from the Advanced Photon Source at Argonne National Laboratory has provided us detailed structural information about the nanowire assemblies and how supramolecular interactions can be leveraged to control their uniformity and domain size.

GP-11 – Band structure study of the optimally doped $BaFe(As_{1-x}P_x)_2$ under continuously tunned uniaxial strain field

Yucheng Guo[1], Zhaoyu Liu[2], Jianwei Huang[1], Ji Seop Oh[1,3], Yichen Zhang[1], Zheng Ren[1], Makoto Hashimoto[4], Donghui Lu[4], Robert J. Birgeneau[3], Jiun-Haw Chu[2], Ming Yi[1]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[2]*Department of Physics, University of Washington, Seattle, Washington, USA*
[3]*Department of Physics, University of California, Berkeley, California, USA*
[4]*Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, California, USA*

Electronic nematicity spontaneously breaking rotational symmetry but preserves translational symmetry have been proposed to play an important role in the unconventional superconductivity in iron-based superconductors (FeSCs). The nematic susceptibility is observed to diverge at the rotational-symmetry breaking transition temperature (Ts), signaling the electronic degree of freedom to be the main driver of the symmetry breaking order. In the global phase diagram, the nematic order can be suppressed by chemical doping before superconductivity appears. The superconducting transition temperature, Tc, reaches maximum when the nematic orders are completely suppressed, where the nematic fluctuations become the strongest [1]. Hence it has been suggested that the nematic fluctuations could play an important role in mediating or enhancing superconductivity. One way to test this proposal is to apply uniaxial strain serving as a conjugate filed of the nematic order which will suppress the nematic fluctuation. Recently, resistivity measurements combined with continuously tunable B_{2g} uniaxial strain in optimally doped $Ba(Fe_{1-x}Co_x)_2As_2$ has revealed an almost complete suppression of T_C [2]. However, the spectral picture behind this suppression is still missing. We use angle-resolved photoemission spectroscopy to study the band structure evolution of optimally doped $BaFe(As_{1-x}P_x)_2$ under continuously tunned uniaxial strain. Our study shows the band response to the uniaxial strain is orbital and momentum dependent. Meanwhile A_{1g} and B_{2g} components of the strain tuned the band structure in different manners.

[1] Nat. Phys. 10, 97–104 (2014)
[2] Nat. Phys. 16, 1189-1193 (2020)

GP-12 – A Dual Catalyst Strategy For Controlling Aluminum Nanocrystal Growth

Christian R. Jacobson,[1] Gang Wu,[6] Lawrence B. Alemany,[1,4] Gopal Narmada Naidu,[2] Minhan Lou,[3] Yigao Yuan,[1,5] Aaron Bayles,[1,5] Benjamin D. Clark,[1,5] Yukun Cheng,[7] Arzeena Ali,[1] Ah-Lim Tsai,[6], Ian A. Tonks,[7] Peter Nordlander,[2,3] and Naomi J. Halas[1,2,3,5]

[1]Department of Chemistry, [2]Department of Physics and Astronomy, [3]Department of Electrical and Computer Engineering, [4]Shared Equipment Authority, and [5]Laboratory for Nanophotonics, Rice University, 6100 Main Street, Houston, Texas 77005, United States

[6]Division of Hematology-Oncology, Department of Internal Medicine, The University of Texas McGovern Medical School, 6431 Fannin Street, Houston, Texas 77030, United States

[7] Department of Chemistry, University of Minnesota—Twin Cities, 207 Pleasant Street SE, Minneapolis, Minnesota 55455, United States

The synthesis of Al nanocrystals (Al NCs) is a rapidly expanding field, but there are few strategies for size and morphology control. Here we introduce a dual catalyst approach for the synthesis of Al NCs to control both NC size and shape. By using one catalyst that nucleates growth more rapidly than a second catalyst whose ligands affect NC morphology during growth, one can obtain both size and shape control of the resulting Al NCs. The combination of the two catalysts (1) titanium isopropoxide (TIP), for rapid nucleation, and (2) Tebbe's reagent, for specific facet-promoting growth, yields {100}-faceted Al NCs with tunable diameters between 35 and 65 nm. This dual-catalyst strategy could dramatically expand the possible outcomes for Al NC growth, opening the door to new controlled morphologies and a deeper understanding of earth-abundant plasmonic nanocrystal synthesis.

GP-13 – Oncogenic KRAS regulates production and surface charge of cancer extracellular vesicles facilitating rapid microfluidic electrophoresis enrichment

Kshipra S. Kapoor[1,2]; Kathleen M. McAndrews[2]; Martin M. Bell[1,5]; Bo Fan[1]; Yi-Lin Chen[4]; Seoyun Kong[2]; Fernanda G. Kugeratski[2]; Lisa S. Biswal[4]; Jacob T. Robinson[1,3,6]; Raghu Kalluri[1,2,3,7]*

[1]*Department of Electrical & Computer Engineering, Rice University, Houston, TX, USA*
[2]*Department of Cancer Biology and Metastasis Research Center, the University of Texas MD Anderson Cancer Center, Houston, TX, USA*
[3]*Department of Bioengineering, Rice University, Houston, TX, USA*
[4]*Department of Chemical & Biomolecular Engineering, Rice University, Houston, TX, USA*
[5]*Applied Physics Program, Rice University, Houston, TX, USA*
[6]*Department of Neuroscience, Baylor College of Medicine, Houston, TX, USA*
[7]*Department of Molecular & Cellular Biology, Baylor College of Medicine, Houston, TX, USA*

Nanosized cancer extracellular vesicles (EVs) exhibit potential to be used for detection of the disease and assessing the treatment response. Although the potential of EV as disease-specific biomarkers is promising, rapid enrichment of cancer EVs remains challenging. Here we show that cancer EVs from patients with pancreatic ductal adenocarcinoma (PDAC) are more anionic when compared to normal EVs. To exploit this property for rapid enrichment of cancer EVs, we developed a Microfluidic ElectroPhoresis (MEP) device, a label-free microfluidic platform. The MEP device's ability to enrich anionic EVs was validated using PDAC cells-derived and serum-derived EVs. We demonstrate that oncogenic KRAS regulates EV production and via phosphatidylserine (PS) induces negative zeta potential on surface of PDAC EVs compared to normal EVs. Genetic extinction of oncogenic KRAS decreased PS levels, induced a cationic shift in the zeta potential of cancer EVs and reduced production of EVs. Overall, this work introduces a MEP device with the capacity for enrichment of circulating PDAC EVs, exploiting its enhanced anionic charge. Such rapid enrichment of oncogenic EVs could be of utility as a biomarker for detection of PDAC.

GP-14 – Electronic Structure of the Substrate Strongly Influences the Self-assembly Behavior of Gold Nano-cubes

Rachael N. Kress,[1] Zhihua Cheng[1] and Matthew R. Jones[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas, United States*
[2]*Department of Materials Sciences and Nanoengineering, Rice University, Houston, Texas, United States*

Nanoparticle self-assembly is a process that is utilized in many different areas of study. One such field is the bottom-up design of materials with unique properties. For this, 2D assemblies are of particular interest. 2D self-assembly involves particles assembling at a liquid-air interface, liquid-liquid interface, or onto the surface of a substrate. There are many different methods by which any of these can be accomplished. In the final case, the chemistries of both the particle and the surface must be considered. The particle-substrate interactions, the particle-particle interactions, the particle-solvent interactions, and the substrate-solvent interactions all must be taken into account when exploring the phase space of 2D self-assembly onto a surface. In previous studies, these interactions are primarily controlled by changing the surface chemistries of the substrate and/or the particles, often by functionalizing these surfaces with ligands. However, the electronic structure of the substrates and its impact on the assembly behavior of the nanoparticles is not often considered.

In this work we present evidence that the electronic structure of the substrate greatly influences the assembly behavior of gold nano-cubes. We explored the assemblies of charged cubes onto substrates with different electronic structures, namely the difference between a substrate made from a gold-coated doped-silicon wafer (a semiconductor) and a gold-coated glass wafer (an insulator). The results showed striking differences in the arrangement, density, and degree of order in the cube assemblies where the only differences in the substrates were the electronic structure.

GP-15 – Plasmonic BIC Arrays as Refractive Index Sensors

Zhichao Li,[1] Ciril Prasad,[1] Xielin Wang,[1] Rosemary Lach[1] and Gururaj Naik[1]

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

Plasmonic sensors have attracted much attention due to their huge nearfield enhancement that leads to high sensitivity. But high nearfield enhancement in nanoscale volumes also leads to high radiative losses which can limit the detectivity. Thus there is a tradeoff between sensitivity and detectivity. The optimum operation of a sensor requires neither the huge sensitivity of plasmonic sensors nor the superb detectivity of photonic sensors. A good compromise between the two extremes is possible by employing the concept of Bound state in the continuum (BIC) in plasmonic sensors. BIC helps in controlling the radiative loss by the array effect and thereby increases the detectivity of plasmonic sensors. Here, we demonstrate a gold nanodisk-based plasmonic structure in a BIC array. By increasing the array period, we show that the quasi-BIC structure allows fine control of the sensitivity and detectivity. Our optimized periodic gold disk structure is fabricated via planar nanofabrication and can detect tiny refractive index shifts from IgG protein at a center wavelength of 650 nm.

GP-16 – Anisotropic Dielectric Function of Aligned Carbon Nanotube Films

Yu-Shuo Liao,[1,2] Jacques Doumani,[2,3] Fuyang Tay,[2,3] Andrey Baydin,[2,4]
Weilu Gao,[5] Shi-Wei Chu,[1,6] and Junichiro Kono[2,4,7,8]

[1] *Department of Physics, National Taiwan University, Taipei, Taiwan*
[2] *Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*
[3] *Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[4] *The Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[5] *Department of Electrical and Computer Engineering, University of Utah, Salt Lake City, Utah, USA*
[6] *Brain Research Center, National Tsing Hua University, Hsinchu, Taiwan*
[7] *Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[8] *Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA*

In the past few decades, carbon nanotubes (CNT) have shown remarkably anisotropic electronic and optical properties as well as exceptional tunability through varying CNT chirality, degree of alignment, and Fermi energy. Recently, several studies have experimentally shown that aligned CNT films display hyperbolic dispersions – i.e., the dielectric constant having opposite signs in different orientations – in the mid-infrared and near-infrared regions of the electromagnetic spectrum, which is caused by strongly polarization-dependent free-carrier absorption and excitonic interband transitions. However, there have been no comprehensive studies on different types of CNT films and existence of hyperbolic dispersion in the ultraviolet region, where CNT response is dominated by π-plasmon absorption. Here, we utilized Mueller matrix ellipsometry and transmission measurements to determine the complex dielectric constant in a wide range of photon energies for different kinds of CNT films, including single- and mixed-chirality films, random and well-aligned films, and films with different Femi energies. We obtained clear evidence of hyperbolic relations in the ultraviolet region for highly aligned CNT films. These results are promising for optoelectronic applications of CNTs films.

GP-17 – Developing pH and Thermal Control of Gold Nanowire Assemblies

David Marolf,[1] Theodor Gerrard-Anderson,[1] and Matthew Jones[1,2]

[1]*Department of Chemistry, Rice University, Houston, Texas 77005, United States*
[2]*Department of Materials Science and Nanoengineering, Rice University, Houston, Texas 77005, United States*

Gold nanowires have gathered interest in recent years for possible applications in the fields of flexible electronics, optics, and catalysis. These applications will require control over the relative positions of the nanowires in aggregations, assemblies, or fully discretized wires. Despite this need, control over nanowire assembly states mostly relies on sheer force alignment and drying effects, with very little attention given to additional supramolecular driving forces (hydrogen bonding, metal chelation, electrostatics, etc.) that enable the high degree of the assembly state of other nanoparticles (spheres, rods, cubes, etc.). This lack of attention is primarily due to difficulty developing reliable methods for functionalizing nanowires with new ligands to enable control over these other supramolecular forces. Our lab has developed a method to functionalize gold nanowires with ligands that terminate in a carboxylic acid functional group. This functional group enables control over the assembly behavior of the nanowires by switching between the neutral, uncharged carboxylic acid and the negatively charged carboxylate. At acidic pH, the nanowires assemble through hydrogen bonding of the carboxylic acids. At basic pH, the carboxylic acid ligands become deprotonated and the functionalized nanowires repel each other electrostatically. Further control of the wires can be maintained through intermediate pHs (where only a percentage of the ligands are deprotonated), electrostatic screening, and heating. These preliminary findings demonstrate that the full supramolecular control available to other gold nanoparticles can be adapted to gold nanowires, vastly increasing the types of applications that can be explored.

GP-18 – Towards the Realization of a Dissipative Phase Transition using a Trapped Ion Quantum Simulator

Abhishek Menon[1], Visal So[1], Midhuna S. Duraisamy[1], Roman Zhuravel[1], and Guido Pagano[1]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, U.S.A.*

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 [1] in the field have predicted the existence of a dissipative phase transition (DPT) in a periodically driven, long-range interacting quantum spin chain between a ferromagnetic ordered phase and a paramagnetic disordered phase as a function of resetting measurement probabilities after coherent evolution. We can probe such rich quantum behavior using our trapped ion quantum simulator. We have developed a high optical access vacuum chamber which houses a linear, 3D, RF blade trap to confine a linear quantum spin chain of Yb^+ ions. Using our 0.3 NA and 0.6 NA re-entrant windows, we facilitate global, tunable Ising type interactions (coherent) to couple spins and individual ion addressing for optical pumping (resetting) , respectively. We report on the latest developments to minimize crosstalk between ions with the individual addressing scheme by achieving $< 2\,\mu$m beam waist per ion, using beam shaping optics and an Acousto-Optic Modulator. We further discuss our plans to decrease the crosstalk through qubit shelving.

[1] Sierant, Piotr et al. Quantum 6 (2022): 638.

GP-19 – Tunable Mid-IR Optical Properties of Al doped ZnO Particles

Adebola Ogundare,[1,5] Christian R. Jacobson,[1,5] Peter Nordlander,[2,3] and Naomi J. Halas*[1,2,3,5]

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

Plasmonic metal nanocrystals (especially Au, Ag and Cu) have attracted significant interests due to their enhanced interactions with electromagnetic radiations and the excitation of free carriers at the metallic surfaces at short wavelength with potential applications in sensing, photocatalysis and energy harvesting. However, potential opportunities abound at longer wavelengths with new class of materials with tunable plasmonic response in the mid-IR. In this project, we explore the controllable colloidal deposition of ZnO on aluminum nanocrystals and aim to achieve aliovalent doping of the ZnO lattices by controlling the synthesis and post-modifications annealing processes.

GP-20 – Enhancing catalytic nitrite hydrogenation via radiofrequency irradiation of magnetic PtFe nanoparticles

Joshua C. Samba,[1, 2] Kiheon Hong,[3] Alison Garrett,[4] Bing Liu,[4] Takao Kurihara,[4] and Michael S. Wong[2, 3]

[1]*Applied Physics Graduate Program, Rice University, Houston, TX, USA*
[2]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[3]*Department of Civil and Environmental Engineering, Rice University, Houston, TX, USA*
[4]*IMRA, Ann Arbor, MI, USA*

Alternating magnetic fields generated from radiofrequency radiation (AMF-RF) can be used to heat magnetic nanomaterials suspended in fluids, enabling the rapid and energy-efficient enhancement of catalytic processes by increasing the surface temperatures of magnetic catalysts (e.g., NiCo, PtFe) directly, instead of indirectly via conventional bulk heating methods (e.g., oven heating, heating jackets). To demonstrate this enhancement effect, catalytic nitrite hydrogenation was performed over PtFe alloy (50:50 nominal wt%) nanoparticles at room temperature and under the influence of AMF-RF heating. At room temperature, PtFe5050 nanoparticles were active for nitrite hydrogenation, achieving an initial reaction rate of 0.11ppm/min and lowering the nitrite concentration by 20% in 2 hours. Under the influence of AMF-RF heating, however, the initial reaction rate for the nitrite hydrogenation increased fivefold, reaching 0.57ppm/min and lowering the nitrite concentration by ~100% in 2 hours, with the bulk temperature post-reaction remaining the same as the initial bulk temperature. This work illustrates the advantages AMF-RF heating has over conventional bulk heating for the enhancement of catalytic reactions.

GP-21 – Ultrasensitive Detection of Oxy-PAHs via Surface-Enhanced Vibrational Spectroscopy

Andrés B. Sánchez Alvarado,[1] Oara Neumann,[2] and Naomi J. Halas[1,2]

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

Surface-enhanced vibrational spectroscopies, specifically Surface-Enhanced Raman Spectroscopy (SERS) and Surface-Enhanced IR Absorption (SEIRA) are techniques that harness the localized surface plasmon resonances to significantly enhance the Raman scattering or infrared absorption of molecules adsorbed on the surface of a plasmonic material. They 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 have been reported. Using substrates consisting of aggregated gold nanoshells (GNS), capable of enhancing both SERS and SEIRA, we studied the detection of polycyclic aromatic hydrocarbons (PAHs) and their oxygen substituted derivatives, known as oxygenated PAHs (oxy-PAHs). These are classes of ubiquitous environmental contaminants well known for their toxicity and carcinogenicity. While unfunctionalized PAHs can be detected and identified by their Raman spectroscopic modes, their oxy-derivatives possess strong IR-active modes, requiring SEIRA detection as well for identification. As test molecules, our studies focused primarily on tetracene and tetracenedione and their SERS and SEIRA spectra. Immobilization strategies using organic monolayers to provide greater affinities for these two aromatic compounds on our SERS and SEIRA substrates are being investigated. In addition, we examined the detection of PAHs extracted from engineered soil samples, to test SERS and SEIRA spectroscopic identification of these types of molecules that may be found as environmental contaminants in real soil samples.

GP-22 – Measuring non-local spatial correlations in quantum gases with ultralong range Rydberg molecules (ULRMs)

S. K. Kanungo,[1,2] Y. Lu,[1,2] C. Wang,[1,2] S. Yoshida,[3] J. Burgdörfer,[3] T. C. Killian,[1,2] F. B. Dunning[1]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[2]*Rice Center for Quantum Materials, Rice University, Houston, Texas, USA*
[3]*Institute of Theoretical Physics, Vienna University of Technology, Vienna, Austria*

The attractive interaction between a Rydberg electron and a nearby ground-state atom can result in the formation of an ultralong range Rydberg molecule (ULRM) at ultracold temperatures. The localized nature of the ground vibrational state in an ULRM can be used to measure non-local spatial correlations in quantum gases, where the excitation rate of a Rydberg dimer and a trimer directly measures the pair correlation[1] and three-body correlation function respectively. The probing distance is tunable by changing the size of the Rydberg molecule, which is controlled by excitation to different principal quantum numbers. In this poster, we present evidence of bunching and anti-bunching in bosonic and fermionic ultracold atom samples respectively that agree with theoretical predictions derived from basic quantum theory.

[1] J.D. Whalen *et al*, Phys. Rev. A 100, 011402(R) (2019)

Research supported by the AFOSR (FA9550-14-1-0007), the NSF (1600059), the Robert A, Welch Foundation (C-0734 and C-1844)

GP-23 – Resolving the rotationally excited states of ultralong-range Rydberg molecules

Yi Lu,[1] Soumya Kanungo,[1] Thomas Killian,[1] Barry Dunning,[1] Shuhei Yoshida[2] and Joachim Burgdörfer[2]

[1] *Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[2] *Institute for Theoretical Physics, Vienna University of Technology, Vienna, Austria*

We report experimental observations of rotational structure in photo-associative spectroscopy of ultralong-range Rydberg molecules (ULRRMs) in an ultracold gas of 86Sr. ULRRM spectroscopy probes scattering wave functions at much larger internuclear separations than does photo-associative spectroscopy to low-lying electronic states [1]. At such separations (Rn≈1400a0 at n=31), the kinetic energy of the initial colliding pairs supports higher partial waves scattering channel, which results in rotationally excited ULRRMs. The rotational structure is further enhanced by the suppression of the s-wave channel due to the near-resonant scattering properties of 86Sr (as=811a0). Results are discussed with the aid of theory that accounts for the recoil momentum associated with photoexcitation, which has proven to lead to transfer of rotational angular momentum to the Rydberg molecules.

GP-24 – Non-Hermitian metasurfaces with non-trivial topology

Ciril Samuel Prasad,[1] Frank Yang,[2] Weijian Li[1], Rosemary Lach[2], Henry Everitt[2,3] and Gururaj V. Naik[2]

[1]*Applied Physics Program, SCI, Rice University, Houston, Texas, USA.*
[2]*Electrical and Computer Engineering, Rice University, Houston, Texas, USA.*
[3]*U.S. Army DEVCOM Army Research Laboratory-South, Houston, Texas, USA.*

Non-Hermitian and topological photonics have been the subject of intense re- search in recent years due to numerous exotic physical phenomena observed in such systems [2, 4]. However, their implementation in nanophotonics is chal- lenging due to poor confinement of light at deep-subwavelength scales. Here, we overcome the limitation to experimentally demonstrate a non-Hermitian meta- surface with nontrivial topology in the k -space [1, 3]. Our hybrid plasmonic-photonic system exhibits an exceptional concentric ring with Z3 topology. We show that our designs open new pathways to achieve directional and wavelength selective thermal emission. These demonstrations unlock quantum many body phenomena in nanophotonics and pave the way towards unconventional light sources at nanoscale.

[1] Chloe F Doiron and Gururaj V Naik. Advanced Materials 31.44 (2019), p. 1904154.
[2] Ramy El-Ganainy et al. Nature Physics 14.1 (2018), pp. 11–19.
[3] Frank Yang et al. Nanophotonics 11.6 (2022), pp. 1159–1165.
[4] Frank Yang et al. Optical Materials Express 11.7 (2021), pp. 2326–2334.

GP-25 – Heteroatom Doped Flash Graphene by Flash Joule Heating

Phelecia Scotland,[1] Lucas Eddy,[1] and James Tour[2]

[1]*Material Science and Nanoengineering, Rice University, Houston, TX, USA*
[2]*Chemsitry, Rice University, Houston, Texas, USA*

Since its discovery, graphene has been hailed as a wonder material due to its extraordinary properties. However, its practical applications have been limited by its zero-band gap, contributing to the lack of catalytic activity. Heteroatom doping substitutes foreign atoms into the graphene lattice which modifies its local structures and electronic states thus allowing for a range of altered optical, electrical, and physical properties. Previously, Tour Group has showed that doped flash graphene (FG) could be achieved by flash Joule heating a mixture of amorphous carbon feedstock with dopant material. Here, we present a post treatment synthesis technique where the dopant material is mixed with turbostratic FG, then flashed Joule heated to form heteroatom doped FG. This process includes two flashes, the first forms turbostratic flashed graphene (FG) and the second achieves the heteroatom functionalization. Here we show the effective doping of single-element FG (nitrogen, boron, and sulfur), two-element co-doped FG (boron and nitrogen) and three element co doped FG (boron, nitrogen, sulfur). This process is solvent free, catalyst, free and utilizes low-cost low toxicity dopants. We observed an increase in the doping percentage by atomic weight of most of the heteroatoms as well as a decrease in interlayer spacing which seems to be a characteristic of the second flash which pushes the layers closer together however, the turbostratic nature of the graphene is still preserved. The electrical energy cost of this method ranges from 1.2 to 10.7 kJ g^{-1} making this process a more improved method compared to previous work.

GP-26 – Single-particle photoluminescence and dark-field scattering during charge density tuning

Emily K. Searles,[1] Stephen Lee, [1] Eric Gomez, [1] Stephan Link*[1,2,3] and Christy F. Landes*[1,2,3,4]

[1]*Department of Chemistry, Rice University, 6100 Main Street, Houston, Texas 77005, USA*
[2]*Smalley-Curl Institute, Rice University, 6100 Main Street, Houston, Texas 77005, USA*
[3]*Department of Electrical and Computer Engineering, Rice University, 6100 Main Street, Houston, Texas 77005, USA*
[4]*Department of Chemical and Biomolecular Engineering, Rice University, 6100 Main Street, Houston, Texas 77005, USA*

When photoexcited, plasmons decay through multiple pathways including surface scattering and photoluminescence. Spectroscopic investigation at the single-particle level can provide insight to decay dynamics. The plasmon's spectral response is sensitive to changes in dielectric environment, charge density, and chemical interface which can be tuned in situ. Electrochemical experiments coupled with dark-field spectroscopy have been shown by our group and others to report on anodic and cathodic charging at the single-particle level, revealing heterogeneity in charge transfer at nanostructured electrodes. While changes in dark-field spectroscopy during the application of charge is well understood, few studies have investigated changes to the photoluminescence of plasmonic nanoparticles under electrochemical charging. The emission of plasmonic nanoparticles may provide a dual sensing platform not accessible through traditional scattering studies by using changes in the interband region to monitor electron charge density tuning and changes in the intraband region to report on plasmon driven processes. In this study, we use correlated single-particle photoluminescence and dark-field scattering to compare the extent of modulation at applied potentials. By using spectral filtration, we conclude that at positive potentials, when electrons are removed from the system, interband photoluminescence decreases as a result of the creation of hotter electrons that can undergo charge transfer into the working electrode. The additional modulation pathway at higher energies offers promise in establishing increased sensitivity and duality to traditional spectroelectrochemical measurements.

GP-27 – Uncovering Domains in Two-Dimensional Ferroelectric SnSe Using Machine-Learning Assisted 4D-STEM

Chuqiao Shi[1], Nannan Mao[2], Jing Kong[2], Yimo Han[1, *]

[1]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX,*
[2]*Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, MA*

Ferroelectric two-dimensional (2D) materials have attracted growing attention because they retain a strong in-plane polarization down to the monolayer limit. Among these 2D ferroelectrics, group-IV monochalcogenides, including SnTe, SnSe, and SnS, contain strongly coupled in-plane ferroelectric polarization and spontaneous lattice strain[1]. In this work, we studied 2D SnSe using a machine-learning-assisted 4D-STEM approach developed in our group[2]. Unsupervised learning uncovers different phases of ferroelectric SnSe, while the subsequent quantitative analysis of the 4D data provides the details in lattice structure. Our method paved the way for a universal workflow for analyzing material deformations using 4D-STEM.

[1] Barraza L.et al. Rev Mod Phys 93, 011001 (2021).

[2] Shi, C. et al. arXiv preprint arXiv:2111.06496, (2021).

GP-28 – RAMBO-II: Ultrabroadband 50-T Magneto-optical Spectroscopy

William Smith,[1] Andrey Baydin,[2,3] Jiaming Luo,[1,4] Hiroyuki Nojiri,[5] Aditya Mohite,[6] Ming Yi,[7] Hanyu Zhu,[1] and Junichiro Kono[1-3,7]

[1]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[3]*Smalley-Curl Institute, Rice University, Houston, TX, USA*
[4]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, TX, USA*
[5]*Institute for Materials Research, Tohoku University, Sendai, Miyagi, Japan*
[6]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[7]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*

The study of a material's optical properties in high magnetic fields is often complicated by the size, construction, and availability of magnets available for optical experiments. The chief aim of the RAMBO: Rice Advanced Magnet with Broadband Optics project is to enable a wide variety of ultrafast and nonlinear spectroscopy measurements not possible or prohibitively difficult in large DC or pulsed magnet systems with the construction of multiple compact, mini-coil-based table-top pulsed magnets with excellent optical access. RAMBO-I has already successfully conducted terahertz (THz) ultrafast spectroscopy experiments in pulsed magnetic fields of up to 30 T, and RAMBO-II will expand these capabilities by not only increasing the maximum field strength but also widening the spectral range into the near infrared (NIR), visible (VIS), and extreme ultraviolet (EUV). The centerpieces of the RAMBO-II expansion are a series of 50-T magnets, which will be the strongest known table-top, repetitive pulsed magnets applied to similar experiments. This presentation features the completed NIR/VIS magnet system along with its experimental capabilities, and some of the plans for the EUV system to be built in the new year.

GP-29 – Exploring the Role of Photosensitizer in Guanine Functionalization of Single-Wall Carbon Nanotubes

Nima Soltani, R. Bruce Weisman*

Chemistry Department, Rice University, Houston, Texas, USA

Single-walled carbon nanotubes (SWCNTs) have attracted a great deal of attention during the past two decades because of their unique optoelectronic properties and their potential applications in biomedical theranostics as well as nanoelectronics. It was recently discovered that it is possible to spatially modulate the exciton band gap of carbon nanotubes through a process known as guanine functionalization. In this reaction, the guanine nucleotides of an ssDNA strand wrapping a nanotube become covalently bonded to sidewall carbon atoms upon exposure to singlet oxygen.[1] In the original work, the authors used xanthene derivatives such as rose bengal and erythrosine B as photosensitizers in order to generate singlet oxygen. It was assumed that this process was an independent step that did not involve the nanotube. However, we have found that rose bengal has a strong tendency to form a charge transfer complex with SWCNTs, and these complexes appear to be essential in the functionalization reaction.

We have studied the complexation through a spectroscopic study of SWCNT fluorescence quenching and the appearance of a charge transfer absorption feature near 600 nm. Both are interpreted as results of nanotube p-doping when the dye adsorbs to the sidewall. We also observe that the charge transfer complex formation accelerates when the rose bengal is optically excited, apparently proceeding through the dye's triplet state. A correlation between extent of guanine functionalization and the concentration of charge transfer complexes is found as ionic strength is changed. We infer that the functionalization reaction is enabled by adsorbed photosensitizers. Interestingly, the extent of SWCNT fluorescence quenching by rose bengal is found to vary significantly with (n,m) structure. This quenching effect therefore provides a simple approach to monitor structure-specific interactions between SWCNTs and coatings, including ssDNA and conventional ionic surfactants.

(1) Zheng, Y.; Bachilo, S. M.; Weisman, R. B. *ACS Nano 13*, 5222 (2019).

GP-30 – Plasmon-Generated Solvated Electrons for Chemical Transformations

David Solti[#,1,2], Kyle D. Chapkin[#,1,3,4], David Renard[1,2], Aaron Bayles[1,2], Benjamin D. Clark[1,2], Gang Wu[5], Jingyi Zhou[1,6], Ah-Lim Tsai[5], László Kürti[2], Peter Nordlander[1,3,6,7] and Naomi J. Halas[1,2,3,6,7]

[1]*Laboratory for Nanophotonics, Rice University; Houston, TX 77005*
[2]*Department of Chemistry, Rice University; Houston, TX 77005*
[3]*Department of Electrical and Computer Engineering, Rice University; Houston, TX 77005*
[4]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University; Houston, TX 77005*
[5]*Department of Internal Medicine, The University of Texas McGovern Medical School; Houston, TX 77030*
[6]*Department of Materials Science and Nanoengineering, Rice University; Houston, TX 77005*
[7]*Department of Physics and Astronomy, Rice University; Houston, TX 77005*

Methods for generating solvated electrons – free electrons in solution – have focused primarily on alkali metal ionization or high-energy electrons or photons. Here we report the generation of solvated electrons by exciting the plasmon resonance of Al nanocrystals suspended in solution with visible light. Two chemical reactions were performed: a radical-addition reaction with the spin-trap 2-methyl-2-nitrosopropane, and a model cyclization reaction with the radical clock 6-bromo-hex-1-ene. A quantum efficiency of at least ~1.1% for plasmon absorbed photon to solvated electron generation can be inferred from the measured radical clock reaction concentration. This study demonstrates a simple way to generate solvated electrons for driving reductive organic chemical reactions in a quantifiable and controlled manner.

[#]*These authors contributed equally.*

GP-31 – Discovery of Charge Density Wave in a Kagome Lattice Antiferromagnet

Xiaokun Teng[1], Lebing Chen[1], Feng Ye[2], Elliott Rosenberg[3], Zhaoyu Liu[3], Jia-Xin Yin[4], Yu-Xiao Jiang[4], Ji Seop Oh[1,5], M. Zahid Hasan[4], Kelly J. Neubauer[1], Bin Gao[1], Yaofeng Xie[1], Makoto Hashimoto[6], Donghui Lu[6], Chris Jozwiak[7], Aaron Bostwick[7], Eli Rotenberg[7], Robert J. Birgeneau[5,8], Jiun-Haw Chu[3], Ming Yi[1], and Pengcheng Dai[1]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[2]*Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA*
[3]*Department of Physics, University of Washington, Seattle, WA, USA*
[4]*Laboratory for Topological Quantum Matter and Advanced Spectroscopy, Department of Physics, Princeton University, Princeton, NJ, USA*
[5]*Department of Physics, University of California, Berkeley, CA, USA*
[6]*Stanford Synchrotron Radiation Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA*
[7]*Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA*
[8]*Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA*

A hallmark of strongly correlated quantum materials is the rich phase diagram resulting from competing and intertwined phases with nearly degenerate ground state energies. A well-known example is the copper oxides, where a charge density wave (CDW) is ordered well above and strongly coupled to the magnetic order to form spin-charge separated stripes that compete with superconductivity. Recently, such rich phase diagrams have also been revealed in correlated topological materials. In two-dimensional kagome lattice metals consisting of corner-sharing triangles, the geometry of the lattice can produce flat bands with localized electrons, non-trivial topology, chiral magnetic order, superconductivity and CDW order. While CDW has been found in weakly electron correlated nonmagnetic AV_3Sb_5 (A = K, Rb, Cs), it has not yet been observed in correlated magnetic ordered kagome lattice metals. Here we report the discovery of CDW within the antiferromagnetic (AFM) ordered phase of kagome lattice FeGe. The CDW in FeGe occurs at wavevectors identical to that of AV_3Sb_5, enhances the AFM ordered moment, and induces an emergent anomalous Hall effect. Our findings suggest that CDW in FeGe arises from the combination of electron correlations-driven AFM order and van Hove singularities-driven instability possibly associated with a chiral flux phase, in stark contrast to strongly correlated copper oxides and nickelates, where the CDW precedes or accompanies the magnetic order.

GP-32 – Titanium oxide improves boron nitride photocatalytic degradation of perfluorooctanoic acid

Bo Wang,[1,2] Kimberly N. Heck,[1,2] Jordin Metz,[2,3] Paul Westerhoff,[4] Pedro Alvarez,[2,3] Michael S. Wong*[1,2,3]

[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX 77005, USA*
[2]*Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment, Houston, TX 77005, USA*
[3]*Department of Chemistry, Rice University, Houston, TX 77005, USA*
[4]*School of Sustainable Engineering and Built Environment, Arizona State University, Tempe, AZ 85281, USA*

Per- and polyfluoroalkyl substances (PFAS), a group of persistent, pervasive, and toxic recalcitrant contaminants, were recently detected in different surface water resources worldwide. Currently, adsorption, which only temporarily sequesters PFAS, is the only method for PFAS remediation, and more efficient destructive technologies are desired. The strong C-F bond makes them hard to be broken down through chemical biological degradation processes, and so efficient water treatment technologies are urgently demanded. We previously discovered that commercial hexagonal boron nitride (BN) photocatalytically degraded perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS) under UV-C (254 nm) illumination using air as oxidant[1,2]. In the present work, I will present follow-up work which extended the wavelength range of the reactivity into the UV-A (365nm light) regime by simply synthesizing BN/TiO_2 composite via calcination for PFAS degradation. PFOA was studied as the PFAS model compound. BN/TiO_2 showed ~15x faster reactivity than TiO_2 according to the PFOA half-lives, while BN was non-active. To understand the unique activity of BN/TiO_2, band diagram analysis will be presented with the assistance of spectroscopy characterizations. A reaction mechanism describing the PFOA degradation will also be discussed according to EPR and radical scavenging experiment results. I will show the PFOA degradation results in salt-containing model water under Houston sunlight. This work presents an effective PFAS destruction approach using a photocatalyst comprised of earth-abundant elements.

[1] Duan, Lijie, et al. Environmental Science & Technology Letters 7.8 (2020): 613-619.
[2] Kim, Minjung, et al. Waste-management Education Research Conference (WERC). Vol. 2. IEEE, 2021.

GP-33 – Super-Mossian dielectrics for nanophotonics

Xielin Wang,[1] Chloe F. Doiron1,[1] and Gururaj V. Naik[2]

[1] *Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, Texas, USA*

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

Refractive index is the defining material property in nanophotonics. High refractive index dielectrics attribute to better light confinement and opens new pathways for applications ranging from broadband metalenses to high-Q-factor resonators. However, there are fundamental limits to the refractive index of any material. The absorption edge and the sub-bandgap refractive index of a semiconductor exhibit a rigid trade-off, popularly known as the Moss rule. However, there are many dielectric materials that surpass the Moss rule, referred to here as super-Mossian dielectrics. We discuss the physical origin of super-Mossian dielectrics to facilitate the search for high index dielectrics. We identify MoS2, a super-Mossian dielectric with index more than 30% higher than the Moss rule prediction. We demostrate the impact of super-Mossian materials on nanophotonics by designing high-Q nanoresonator arrays using MoS2.

GP-34 – Light tunability of 1T-TaS2 and non-local medium analysis

Ding Zhang,[2] Gururaj Naik[1]

[1] *Electrical & Computer Engineering, Rice University, Houston, TX, United States*
[2] *Physics & Astronomy, Rice University, Houston, TX, United States*

Strongly correlated electron systems possess a complex energy landscape and host many interesting quantum phenomena, such as charge density wave (CDW). CDWs have been widely observed in quasi-2D materials, including transition metal dichalcogenides (TMD) and cuprates. Among them, 1T-TaS2 exhibits an incommensurate CDW at room temperature. A past study from our group has revealed this material's tunability along the c axis under the illumination of incoherent white light. In this study, furthering the said investigation, we also discover the tunability perpendicular to the c axis for this material. We then analyze the dielectric function based on reflection data and employ a non-local model to account for the influence of domain sizes on electron susceptibility. The cause of this light tunability is related to the stacking configurations of the 2D domains of the system. In the future, we want a density functional theory calculation to help reveal more details about this mechanism.

GP-35 – Single particle chirality studies of DNA-templated AuNR dimers for detailed structural and mechanistic insights

Amrita Chakraborty,[1] Mihir Dass,[2] Tim Liedl,*[2,] Stephan Link*[1,3,4]

[1]Department of Chemistry, Rice University, Houston, TX, 77005 USA. [2]Faculty of Physics and Center for NanoScience (CeNS), Ludwig-Maximilians-University, 80539 Munich, Germany. [3]Smalley Curl Institute, [4]Department of Electrical and Computer Engineering, Rice University, Houston, TX, 77005 USA.

Directing the assembly of plasmonic nanoparticles into chiral superstructures has diverse applications including chiroptical sensing, nonlinear optics, and biomedicine. DNA nanotechnology, due to its programmability, enables precise placement of nanoscale objects such as plasmonic nanoparticles, biological materials such as antibodies, enzymes and proteins. Specifically, DNA origami has emerged as an elegant tool to construct chiral structures using nanoparticles that exhibit strong optical signal in the visible region. However, the sensitivity of ensemble circular dichroism (CD) spectroscopy is severely limited due to sample heterogeneity as it only measures average values. Besides, in case of plasmonic nanoparticles with non-negligible scattering intensity, the standard transmission spectroscopy typically measures the differential extinction instead of differential absorption. However, in a dark-field optical setup, differential scattering of nanostructures can be isolated from differential absorption. Investigation of chirality at the single particle level in such a setup not only provides detailed mechanistic insights associated with the individual nanostructures but also has potential to lower the detection limit of chiral biomolecules to the single molecular level. Recently, circular dichroism scattering (CDS) spectroscopy on single chiral assemblies made of gold nanorods (AuNRs) has led to important findings. One such study from our group has quantified the effects of size-mismatch between the constituent AuNRs and large twist angles on the resulting circular differential scattering spectrum.[1] Another important study has revealed that BSA mediated chiral aggregates of AuNRs and just a few proteins in interparticle gaps of achiral assemblies are responsible for the ensemble signal, but single nanoparticles do not contribute.[2] In the current work, we study the DNA-origami mediated AuNR-dimer with left handed structural twist which shows gigantic ensemble CD signal. By performing a single particle chirality study, namely CDS spectroscopy, on this simple yet highly precise chiral nanostructure, we aim to address a few fundamental questions:

1. What additional information do the single particle CDS provide compared to ensemble CD?
2. What is the effect of orientation of the nanostructures with respect to the substrate on their chiral signal?
3. What is difference between using free space polarized light and interface confined electromagnetic waves generated by total internal reflection (TIR) with respect to the measured line shape and signal intensity of the chiral nanostructures?

We observed an important aspect of CDS. So far, the CDS studies have been performed in the total TIR mode, where the particles were excited by an evanescent field. Here, we excite the nanostructures by circularly polarized light incident on them at a high angle and observed that in this case the CDS signal shows an opposite sign compared to that obtained in the TIR mode. Together with correlated electron microscopy of the nanostructures and theoretical modelling, this observation contributes to deeper understanding of plasmonic CD.

1. Wang, L. Y.et al., Circular Differential Scattering of Single Chiral Self-Assembled Gold Nanorod Dimers. *ACS Photonics* **2015**, 2, 1602−1610.
2. Zhang, Q. et al., Unraveling the origin of chirality from plasmonic nanoparticle-protein complexes. *Science* **2019**, 365, 1475–1478.

GP-36 – Flash Joule heating: A new energy-efficient thermal technique for critical materials recovery and waste management

Bing Deng[1], and James M. Tour[1]

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

Precious metal recovery from electronic waste, termed urban mining, is important for a circular economy. Present methods for urban mining, mainly smelting and leaching, suffer from lengthy purification processes and negative environmental impacts. Here, a solvent-free and sustainable process by flash Joule heating is disclosed to recover precious metals and remove hazardous heavy metals in electronic waste within one second. The sample temperature ramps to ~3400 K in milliseconds by the ultrafast electrical thermal process. Such a high temperature enables the evaporative separation of precious metals from the supporting matrices, with the recovery yields >80% for Rh, Pd, Ag, and >60% for Au. The heavy metals in electronic waste, some of which are highly toxic including Cr, As, Cd, Hg, and Pb, are also removed, leaving a final waste with minimal metal content, acceptable even for agriculture soil levels. Urban mining by FJH would be 80× to 500× less energy consumptive than using traditional smelting furnaces and more environmentally friendly.

GP-37 – Photoluminescence Properties and $g^{(2)}$ Correlation Measurements of Aligned Carbon Nanotube Quantum Emitters

Manukumara Manjappa,[1] Jacques Doumani,[1,3] Vanessa B. Espinoza,[4] Xinyue Li,[2] Kazuhiro Yanagi,[5] Weilu Gao,[6] R. Bruce Weisman,[4] and Junichiro Kono[1,2,7,8]

[1]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[2]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[3]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, TX, USA*
[4]*Department of Chemistry, Rice University, Houston, TX, USA*
[5]*Department of Physics, Tokyo Metropolitan University, Tokyo, Japan*
[6]*Department of Electrical and Computer Engineering, University of Utah, Salt Lake City, UT, USA*
[7]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA*
[8]*The Smalley-Curl Institute, Rice University, Houston, TX, USA*

Covalently functionalized single-wall carbon nanotubes (SWCNTs) have shown great prospects as tunable solid-state single-photon emitters in the near-infrared wavelengths capable of operating at room temperature. Here, we aim to study the collective excitation and emission properties of single-photon emitters in a macroscopically and periodically ordered ensemble of quantum defects in SWCNTs. We used sodium deoxycholate surfactant to disperse CoMoCAT SWCNTs that were covalently functionalized through photoexcitation of sodium hypochlorite (NaClO) under oxygen-free conditions to introduce quantum defects. We explore novel fabrication approaches to achieve macroscopically ordered defect sites in the functionalized nanotubes in order to enhance the photoluminescence intensity and thereby high single photon emission rates that are otherwise strongly quenched due to the sensitivity of the SWCNTs to the dielectric environment and intense laser excitation. We study their emission properties through photoluminescence excitation, polarization and photon auto/cross-correlation measurements to probe the effect of collective quantum emission from the array of emitters on the photon lifetime and single-photon purity.

GP-38 – Field induced Lifshitz spin liquids in frustrated magnets

Shouvik Sur,[1] and Andriy H. Nevidomskyy[1,2]

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

Frustrated magnets support a variety of magnetically ordered phases. Along the boundaries separating these phases long-range magnetic orders are usually suppressed, which may lead to the stabilization of spin-liquid states. Here, we study magnetic field driven transitions in frustrated magnets in the vicinity of the aforementioned phase boundaries. We demonstrate that along the phase boundaries transitions to field-polarized states are described by the Lifshitz universality class, and obtain exact critical exponents. At sub-critical fields, strong quantum fluctuations prevent magnetic long-range orders, and stabilize algebraic liquids that are reminiscent of one-dimensional Luttinger liquids. We also draw connections between the Lifshitz field theories discussed here and rank-2 U(1) gauge theories.

GP-39 – Plasmonically Enhanced Hydrogen Evolution with an Al-TiO_2-based photoelectrode

Lin Yuan[1, 2, 5], Anvy Kuriakose[3, 5], Jingyi Zhou[4, 5], Hossein Robatjazi[1, 5], Peter Nordlander[2, 3, 4, 5], and Naomi J. Halas[1, 2, 3, 5]

[1] Department of Chemistry, Rice University, Houston, Texas 77005, United States
[2] Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, United States
[3] Department of Physics &Astronomy, Rice University, Houston, TX, USA
[4] Department of Materials Science and Nanoengineering, Rice University, Houston, Texas 77005, United States
[5] Laboratory for Nanophotonics, Rice University, Houston, Texas 77005, United States

Photoelectrochemical water splitting, as a method for producing clean Hydrogen, could benefit both from plasmon-enhanced processes and the incorporation of earth-abundant materials in photoelectrode design. Here we report a n-TiO_2/Aluminum (Al) nanodisk/p-GaN photoelectrode sandwich device that exhibits enhanced H_2 generation efficiencies due to a combination of plasmon-enhanced processes. Hot electrons generated in the illuminated Al nanodisk are injected into the conduction band of the TiO_2 layer, subsequently transferring into water molecules adsorbed on the TiO_2 surface, driving H_2 evolution. The photocurrent densities we observe are nearly an order of magnitude higher than in an equivalent device with the Al nanodisk replaced by a Au nanodisk of the same size, and are on par or better than previous reports of plasmonic photoelectrodes using Au nanoparticles in combination with co-catalyst species.

Poster presentations: undergraduate students

UG-1 – Colorimetric detection of metal ions in water

Emily B. Aspey,[1] Joshua C. Samba,[1, 2] and Michael S. Wong[1,3]

[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*
[2]*Applied Physics Graduate Program, Rice University, Houston, TX, USA*
[3]*Department of Civil and Environmental Engineering, Rice University, Houston, TX, USA*

Transition metal catalysts are a very popular water treatment technology for several reasons, including their ability to enhance reaction rates and their high reduction potential. However, when these catalysts experience issues with their stability or are exposed to incompatible chemicals, metal ions can be released into the solution, causing metal leaching. Current methods to detect metal ions in water (e.g., ICP-MS and TEM) are extremely expensive and require multiple hours or days of analysis to get results. This demonstrates the need for a quick, cheap method for detecting the presence of metal ions in water. A group at ASU found a solution to this problem, designing a “catalytic reactivity to nanoparticle” assay (CRNP) which uses a dry powder containing methylene blue (MB) and sodium borohydride ($NaBH_4$) to rapidly (2 min) detect metallic nanoparticles in water. Our group at Rice used a simplified version of this assay to rapidly detect the presence of metal ions in water using UV-Vis spectroscopy by comparing the initial reaction rates of waters containing various amounts of metal ions. Methylene blue was reduced by hydrogen gas produced by sodium borohydride in the presence of Fe (III) ions at concentrations ranging from 0ppb - 750ppb. As the concentration of Fe (III) ions increased, we observed an increase in the initial reaction rate. This technique is a quick and simple way to ensure that the waters we treat are cleaner than how they started.

UG-2 – Temperature-responsive polymer-grafted carbon nanotubes for active control of mineral scaling in wastewater filtration

Michelle Chen[1, 2], Xiaoyin Tian[1], Yifan Zhu[1], Jun Lou[1]

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

Clean water is essential to all communities, especially amidst the water scarcity crisis, which impacts billions around the world. During wastewater treatment, filters used for membrane separation can become damaged by scale deposition when mineral solids accumulate to obstruct pores of the filter. Here, we present a novel solution to overcome the scaling problem using self-cleaning carbon nanotube (CNT)/polymer composite-coated membranes, which have high electrical conductivity, excellent hydrogen evolution reaction (HER) performance, relatively low cost, and potential to be easily modified. We hypothesize that because the temperature-responsive polymer poly-N-Isopropylacrylamide (PNIPAM) swells and contracts upon temperature fluctuations, it would result in the removal of scale deposits. To test this hypothesis, CNTs were first grown in situ on carbon paper using chemical vapor deposition (CVD) furnace growth. The CNTs were found to reduce scale deposition on the membrane compared with pure carbon paper. Subsequently, PNIPAM was uniformly synthesized on the CNT using surface-initiated activators regenerated through electron transfer (ARGET) atom transfer radical polymerization (ATRP). Fourier-transform infrared spectroscopy (FT-IR) and X-ray photoelectron spectroscopy (XPS) measurements confirmed the successful anchoring of PNIPAM onto CNTs. Unlike pristine CNTs, CNTs coated with PNIPAM exhibited hydrophilic properties at room temperature, with a contact angle much smaller than 90° after 30 seconds. At 35°C, above its lower critical solution temperature (LCST) of 32°C, its contact angle was larger than 90° after 30 seconds, demonstrating its hydrophobic properties at higher temperatures. To further confirm our hypothesis, we will explore the anti-scaling performance of PNIPAM-coated CNTs when shifting temperature.

UG-3 – Effects of Doping Processing Conditions on Carbon Nanotube Fiber Specific Electrical Conductivity

Christopher Connolly, Mitchell Trafford, Matteo Pasquali

Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA

Carbon nanotube fibers (CNTFs) are a versatile material that possess properties including low density, high mechanical strength, high thermal conductivity, and high electrical conductivity. These properties are desirable for industries such as aerospace and automotive because of their potential use as lightweight electrical wiring. Improving the electrical conductivity of CNTFs will further improve their ability to displace conventional conductors like copper. This can be achieved by incorporating chemical species into the fiber, a process known as doping. Our research team experimentally studied the effects that doping processing conditions had on CNTFs, with the aim to increase specific electrical conductivity by lowering electrical resistivity while maintaining a low fiber mass. Using iodine monochloride (ICl) as a p-type dopant, our team studied the effects of various pressures, temperatures, and concentrations of dopant on the efficacy of dopant incorporation into the CNTFs. The doping efficacy was evaluated using linear density and 4-wire resistance measurements, allowing us to calculate the specific electrical conductivity of the doped CNTFs. Our preliminary tests show that doping CNTFs with ICl can increase specific electrical conductivity by upwards of 10%.

UG-4 – Shape Classification of Gold Nanotriangles using Spectrally Trained Machine Learning Model

Haoyu Joshua Fan,[1] Katsuya Shiratori,[1,2] Alexander Al-Zubeidi,[1] Thomas Heiderscheit,[1] and Stephan Link [1,3,4]

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

Gold nanotriangles (AuNTs) are anisotropic nanoparticles that exhibit various properties based on shape/size such as large surface-to-volume ratio and a size-relative absorption peak. They are useful in photocatalysis, surface-enhanced spectroscopic techniques, and other photothermal applications. The synthesis method achieves up to around 95% at the batch level after purification. Still, at the single particle level, the synthesis rarely removes byproducts such as hexagonal plates and decahedrons. Therefore, there is no option but to use electron microscopy and correlation techniques of nanoparticles in order to observe optically-measured characteristics, which can be time-consuming and often destructive to the samples. Here we show that machine learning models can classify the shape of AuNTs from spectra alone in real time, which is more accessible and efficient. We trained logistic regression and decision tree models with a dataset of 250 AuNTs. When validated with a testing dataset, the decision tree model consistently classified AuNTs with an accuracy of about 94%, while the logistic regression struggled. With further testing, we found that the decision tree model can consistently classify AuNTs after being trained on approximately 110 nanoparticles. Our findings strongly support the use of machine learning to classify the shape of AuNTs and even other nanoparticles.

UG-5 – Everlasting Multiplexed Inertial Coalescence Filters to Address Environmental Challenges

Damian Gonzalez,[1] Rawand Rasheed,[1] & Daniel J. Preston[1]

[1] *Department of Mechanical Engineering, Rice University, Houston, Texas, United States*

Water scarcity presents a major modern-day issue, with increased water costs posing a significant problem for cost effectiveness of cooling towers used in industrial cooling. This work describes everlasting multiplexed inertial coalescence filters composed of parallel helical pathways that are additively manufactured with features used to drain captured liquid. These filters are designed to filter fine droplet streams (<20 μm). Filter drain rates were characterized as a function of applied pressure using liquids of varying viscosity for filters with varying porous medium infill densities. Experimentally measured filter drain rates were in good agreement with a model based on Darcy's law. Everlasting multiplexed inertial coalescence filters were implemented in experimental setups for cooling tower water recovery and carbon dioxide capture demonstration. The implications of our work include process intensification in liquid-gas chemical processes, lunar dust filtration, and carbon dioxide scrubbers in spacecraft and naval vessels.

UG-6 – Dynamic Control of Energy Transfer in AuNR-PANI Hybrids through pH Change

Annette Jones[1], Emily K. Searles[1], Martin Mayer[2], Marisa Hoffman[2], Andreas Fery[2], Stephan Link*[1,3,4], Christy F. Landes*[1,3,4,5]

[1]*Department of Chemistry, Rice University, 6100 Main Street, Houston, Texas 77005, United States*
[2]*Leibniz-Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry and Polymer Physics, Dresden, Germany*
[3]*Smalley-Curl Institute, Rice University, 6100 Main Street, Houston, Texas 77005, United States*
[4]*Department of Electrical and Computer Engineering, Rice University, 6100 Main Street, Houston, Texas 77005, United States*
[5]*Department of Chemical and Biomolecular Engineering, Rice University, 6100 Main Street, Houston, Texas 77005, United States*

Plasmonic nanoparticles support a localized surface plasmon resonance and large cross-section, allowing unmatched light absorption into confined areas; however, the ultrafast lifetime of plasmon decay presents challenges in harnessing the energy before it dissipates into heat. Hybridization of plasmonic nanomaterials with energy transfer acceptors such as semiconductors enables subsequent reactions to harness the energy offered from plasmonic nanomaterials. Energy transfer into interfacial material can be measured through plasmon damping, which is observed in the scattering of individual gold nanorods upon the addition of a polyaniline shell. Polyaniline is sensitive to pH changes, transitioning from emeraldine salt to pernigraniline base as pH increases. In this study, gold nanorod-polyaniline (AuNR-PANI) hybrids are investigated in different pH environments to determine optimal conditions for the efficient transfer of energy from the plasmon to the PANI shell. Using a microfluidic cell on an inverted hyperspectral dark-field microscope modulations in resonance energy and linewidth due to changes in the refractive index and plasmon dynamics, respectively, can be monitored for individual particles across pH conditions. As the pH varies, the PANI absorption spectra shift resultant from the change in protonation state. Broader linewidths, indicating a faster plasmon decay time, are seen to be resonance energy dependent. Energy transfer is most efficient when there is the most overlap between AuNR scattering and PANI absorption allowing pH mediated control over energy transfer efficiency.

UG-7 – The Effect of Exosomes Surface Charge on Drug Delivery Applications

Seoyun Kong,[1] Kshipra Kapoor,[2,3] and Raghu Kalluri[3,4,5]

[1]*Department of Materials Science and Nanoengineering, Rice University, Houston, TX*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX*
[3]*Department of Cancer Biology, The University of Texas MD Anderson Cancer Center, Houston, TX*
[4]*Department of Bioengineering, Rice University, Houston, TX*
[5]*Department of Molecular and Cellular Biology, Baylor College of Medicine, Houston, TX*

Exosomes are nano-sized extracellular vesicles secreted by all cell types, which recently gained significant attention in the scientific field due to their ability to act as cargoes for proteins, metabolites, and nucleic acids to recipient cells, thus facilitating intercellular communication. This intrinsic property has revealed their potential utility as biomarkers and uses in precision medicine in many diseases, including cancer. While the exosomes' biomolecular properties are being actively studied, little is known about their electrical properties and how they affect their body function. Zeta potential, the measure of effective surface charge on the nanoparticle's surface, is a promising method for studying the activity of exosomes in biological processes. Substantial studies have shown that the surface charge of particles regulates the particles' in-vivo fate and plays a vital role in the interactions of nanoparticles with biological components. However, limited studies investigated the relationship between the zeta potential of exosomes and their drug delivery efficacies. In this study, exosomes were isolated from different FDA-approved cell lines and tagged with lipids of cationic, anionic, and zwitterionic charges to study the effect of surface charge on drug-loading efficacy. We employed mechanical methods for permeabilizing the exosomes' membrane, such as sonication and electroporation, to load our small molecules (siRNAs). Then, the siRNA-loading efficiencies of exosomes were quantified by comparing the mean fluorescence intensity before and after siRNA uptake. Understanding the relationship between the zeta potential of exosomes and their drug delivery efficacies will improve the potential therapeutic control of biological nanoparticles in the human body.

UG-8 – Numerical Simulations of Spin-boson System with Trapped Ions

Mingjian Zhu[1], Guido Pagano[1], Roman Zhuravel[1]

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

Direct simulation of open quantum many-body systems can be realized by atomic quantum simulators based on trapped ions with carefully engineered dissipative processes. This project serves as a pilot study for quantum simulation experiments to be done in the future. It aims to explore appropriate parameter ranges for our simulator and gain prior insights into possible outcomes. We examine time evolution of trapped ion systems with distinctive setups by performing numeric integrals to solve the master equation. The first part of this project involves simulation using the complete time-dependent Hamiltonian of a 1-D chain of N ions including a full treatment of both spin and phonon degrees of freedom. The second part focuses on realistic chemical physics problems. We first consider a 2-ion system which is well-studied as a simulator for electron transfer [1] to benchmark our method. Then, we investigate the evolution of a 3-ion system used to simulate excitation transfer. We locate a few peaks of transfer rate and steady state population imbalance as a function of site energy imbalance. The physics that determines the peak positions will be further explored.

[1] Schlawin, Frank, Manuel Gessner, Andreas Buchleitner, Tobias Schätz, and Spiros S. Skourtis. *PRX Quantum* 2, no. 1 (2021): 010314.

UG-9 – The effects of hydrogen bonds on Raman active vibrations in flavonoids

Charles Pacheco[1], Campbell Uyeki[1], Mathieu Simeral[1], and Jason Hafner[1]

[1]Physics, Rice University, Houston, Texas, United States

The Raman spectra of two flavonoids, flavone and quercetin, were investigated through comparisons between spectra recorded from pure powders and spectra calculated with time dependent density functional theory (TDDFT). For both flavone and quercetin, 17 peaks were assigned to specific molecular vibrations. Both flavonoids were found to have a split peak between 1250 – 1350 cm^{-1} that is not predicted by TDDFT calculations on isolated molecules. In each case it was shown that the addition of hydrogen bonded molecules, arranged based on crystal structures, explained the split peaks. These peaks were due to stretching of the bond between the benzopyrone and phenyl rings and represent a characteristic spectral feature of the flavonoids. Spectra of pollen grains from *Quercus virginiana* were also recorded and exhibit several peaks that correspond to the quercetin spectrum. May present elements of additional works underway.

ECE-1 – Visualize the Data Collected in Agora Experiments by showing them into Figures

Luckner Ablard, Oscar Bejarano, Di Mu

Electrical and Computer Engineering, Rice University, Houston, Texas, USA

Agora is a real-time massive MIMO baseband software framework used for wireless research. Researchers make use of the Agora system to conduct custom experiments and to analyze different metrics such as throughput, bit error rate (BER), and signal-to-noise ratio, among others. In this project we develop a set of software functions, in Python, to parse and visualize the data files produced with Agora by showing them into figures. Researchers spend most of their time preparing and collecting data for analysis. We process CSV files that contain data reports on multiple columns and rows. One of the first important step to search or retrieve data from CSV files is limited due to their format. The research consists of the following methods for analyzing data in Agora and other related fields such as supporting data input from standard input stream, gathering the data of different parameters, and feeding the data into plots and allowing customized plot settings.

ECE-2 – Simulated study of LG-OAM Link Security using Antenna Arrays

Gabriel Baquero,[1] Dr. Chia-Yi Yeh[1], Dr. Edward Knightly[2]

[1]*Rice Networks Group, Rice University, Houston, Texas, United States*

The application of Orbital Angular Momentum (OAM) beams in wireless communication is a relatively new area of study. Unlike conventional transmissions with a plane wavefront, OAM beams feature a helical wavefront and require different receiving architectures to decode the transmitted signal. This research studies the capabilities of eavesdropping on wireless communication systems using OAM. Demonstrating that eavesdropping has a low impact on OAM link security by simulating a Laguerre-Gaussian beam capable of carrying OAM and using different eavesdropping locations to analyze the receiving capabilities of each configuration. The research also provides valuable insight into designing and manufacturing antenna array hardware using computer design software and 3D printing techniques.

ECE-3 – Massive MIMO Radio Network Programming of Client-Server Models

Matthew Bohr[1], Summer Brandon[2]

[1]*Electrical Engineering, The College of New Jersey, Trenton, New Jersey, United States*
[2]*Computer Engineering, Prairie View A&M University, Prairie View, Texas, United States*

Rice University's Agora platform [1] is a massive multiple-input multiple-output (mMIMO) real-time baseband processing framework. It pushes the limits of traditional MIMO wireless systems by exploiting a many-antenna array to enable multiple concurrent radio links and to increase the overall network capacity. Agora runs on a Linux-based host machine that communicates with massive MIMO hardware via SoapySDR, an open source generalized API and runtime library for interfacing with SDR devices. The communication between the hardware and Agora uses short 1500-byte UDP packets. Given that each packet has a header and offset check, such short packets lead to a large processing overhead. To reduce this overhead and to increase system performance, we want to extend the Agora software framework to add 9000 MTU support. Our research focuses on a shortcoming with SoapySDR, in which an MTU of 9000 causes packets to go missing between the hub and hardware. To resolve this, we utilized the open-source network packet analyzer software known as WireShark to uncover the root of these issues. In addition to this, we developed both UDP and TCP client-server models and modified the Agora software to allow network traffic to alternate between IPv4 or IPv6 addresses. This research provided insight into the ways in which software based mMIMO systems communicate with hardware. Future research entails resolving the MTU size conflict to prevent the radio network from crashing when the size is set to 9000.

[1] Jian Ding, Rahman Doost-Mohammady, Anuj Kalia, and Lin Zhong. 2020. Proceedings of the 16th International Conference on emerging Networking EXperiments and Technologies. Association for Computing Machinery, New York, NY, USA, 232–244.

ECE-4 – Behavioral Modeling of Monkeys in Virtual Reality Foraging using Reinforcement Learning

Siyi (Cici) Du, Xaq Pitkow, Yizhou Chen, Ruiyi Zhang, Dora Angelaki

Department of Neuroscience, Baylor College of Medicine, Houston, Texas, US
Department of Electrical and Computer Engineering, Rice University, Houston, Texas, US

While traditional neuroscience tasks often only demonstrate basic cognitive functions like perception, tasks that show higher cognitive functions such as planning and memory are relatively rare. The firefly task is a continuous virtual-reality foraging task in which animals receive juice rewards by catching "fireflies" that flash on and off. The task is interesting enough to exhibit more advanced functions of the brain, as it requires animals to use ambiguous sensory data, memory, and predictions. Analyzing behavioral data of monkeys in the task can shed light on their cognitive strategies and brain functions. After a descriptive analysis, we trained a reinforcement learning agent to model monkeys' behaviors using soft actor-critic (SAC) algorithm and long short-term memory (LSTM) neural network. By watching animation of monkeys' performance in the task, we observe several interesting patterns, which we use to both characterize the monkeys' behaviors and compare them with those of the reinforcement learning agents. We found that the RL agent closely resembles the monkeys in some measurements and yet functions better in others, suggesting that the monkeys have greater internal noise than the RL agent. For further analysis, different noises can be added to the RL agent to find the model that best explains the monkeys' behaviors.

ECE-5 – UnoNet: Graph Neural Networks for wireless networks modeling

Timofey Efimov,[1] Santiago Segarra,[1] Abhishek Kumar, [1] and Jose Cortes[2]

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

[2]*Department of Mathematics, University of Texas, Arlington, Texas, United States*

Digital twin is a new promising idea in network modeling, which enables to achieve efficient operation in Software-Defined Networks. Each wireless networks has a set of Key Performance Indicators (KPIs) which define its quality, and include delay, jitter, and throughput. However, it is hard to predict those KPIs accurately and do it computationally efficient before building the actual network. The proposed solution is to create a digital twin of the network and use Graph Neural Network (GNN) based model, called UnoNet, to predict these KPIs with high accuracy and in a timely manner. The model considers topology of the network, routing scheme, and traffic through the network to predict the network indications, and utilizes node, edge, and path information to make the predictions accurate. Choice of GNNs is justified by its ability to learn graph-structured information much better than other neural network architectures, and generalize to unseen topologies, routings, and traffic intensities. In this project, we have compared the performance of the proposed model to other neural network-based approaches to demonstrate its ability to make accurate, fast, and generalized predictions. With UnoNet, it is possible to achieve efficient routing and network planning prior to physically building the network.

ECE-6 – Aerial Drone Positioning and DOA estimation using Massive MIMO array

William ‘Nat’ Hill, Tylor Gonzalez, Tarence Rice, and Edward W. Knightly

Electrical and Computer Engineering REU, Rice University, Houston, Texas, USA

Determining the Angle of Arrival(AoA) in-air lacks extensive study, and so we have combined both the ASTRO drone platform and RENEW M-MIMO platform to expand on their capabilities to measure and estimate/track the Angle of Arrival (AoA) within 3D space. More specifically, five questions are presented in order to challenge and analyze the performance of all technologies involved. To accompany the questions, multiple parameters were considered and tested such as gain, polarity of antennas, SDR health, companion computers, location, multipath, and different AoA methods. The results of this research were conducted under loosely strict real world scenario studies of uniform antennas set up in a 5x8 base station with uniform spacing. An Iris SDR is used in-air to scan a particular angular region of interest, and through these two setups both the azimuth and elevation angles can be measured, afterwards we use a variety of AoA algorithms but primarily Matlab’s own Beamscanning “Phased Array System Toolbox”. Shown is the performance and interpretation of collected data according to our research questions.

ECE-7 – Finding Patterns in Food Webs due to Biome and Environment Variables

Zachary Katz[1], César Uribe[1], Lydia Beaudrot[2]

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

The motivation for research was that we could find a way to measure 'distance' between food webs so that we could better understand how environment variables and human urbanization both affect the structure and resilience of food webs. The issue is relevant today because urbanization and pollution sometimes negatively deteriorate food webs and our research could help us detect those changes in food webs. Our research attempts to find how similar different food webs are to each other, so that differences in environment can be used to explain the differences in food webs. The scope of our research includes locations across biomes in sub-Saharan Africa. Our approach was to use Python to read in the food web data from an Excel spreadsheet and then store it in text files. Then, we created diagrams of each food web so that we could get a rough sense of how each food web was structured. Then, we created a matrix of Gromov-Wasserstein distance between each pair of food webs and used the Gromov-Wasserstein distance to judge how different food webs in different biomes are to each other. Our results were that food webs from the Deserts and Xeric Shrublands biome were significantly farther away from every other biome than food webs from other biomes were to each other. Also, the difference in richness of food web locations, and to a lesser extent the geographical distance, was significantly correlated with the Gromov-Wasserstein distances between food webs.

ECE-8 – Ultrastrong Coupling of Electron Paramagnetic Resonance and Fabry–Pérot Cavity Modes in Gadolinium Gallium Garnet

Jae Joon Lee,[1] Elijah Kritzell,[2,3] Fuyang Tay,[2,3] Andrey Baydin,[2,4] and Junichiro Kono[1,2,4,5]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, Texas, USA*
[3]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[4]*Smalley-Curl Institute, Rice University, Houston, Texas, USA*
[5]*Department of Material Science and NanoEngineering, Rice University, Houston, Texas, USA*

Cavity quantum electrodynamics in condensed matter have recently emerged as an exciting new subfield of physics, bridging the traditional fields of quantum optics and many-body condensed matter physics. Powerful light–matter coupling can lead to nonintuitive modifications of electronic states in materials, which can be probed through optical, electronic, thermal, or magnetic measurements. In particular, when the system enters the ultrastrong coupling regime where the coupling strength becomes comparable to the bare frequency of the cavity mode, many exotic properties can emerge because standard approximations and assumptions in light–matter interactions break down. Here, we investigated electron paramagnetic resonance (EPR) in gadolinium gallium garnet (GGG), a paramagnetic insulator, and observed ultrastrong coupling between EPR and Fabry-Perot (FP) cavity modes. The measurements were done using RAMBO (Rice Advanced Magnet with Broadband Optics), which combines a high magnetic field of up to 30 T and a single-shot terahertz time-domain spectroscopy. The resonant condition between EPR and a FP cavity mode was met at ~17 T by polishing the GGG sample to about 180 μm. The measured normalized coupling strength reached 0.13 at 95 K and 0.1 at 250 K. The results are promising to pursue cavity materials engineering in this system.

ECE-9 – Preparation and Characterization of Carbon Nanotube Quantum Emitter Assemblies

Xinyue Li,[1] Jacques Doumani,[2,3] Manukumara Manjappa,[2] Vanessa Espinoza,[4] Kazuhiro Yanagi,[5] Weilu Gao,[6] R. Bruce Weisman,[4] and Junichiro Kono[1,2,7,8]

[1]*Department of Physics and Astronomy, Rice University, Houston, TX, USA*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA*
[3]*Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, TX, USA*
[4]*Department of Chemistry, Rice University, Houston, TX, USA*
[5]*Department of Physics, Tokyo Metropolitan University, Tokyo, Japan*
[6]*Department of Electrical and Computer Engineering, University of Utah, Salt Lake City, UT, USA*
[7]*Department of Materials Science and NanoEngineering, Rice University, Houston, TX, USA*
[8]*The Smalley-Curl Institute, Rice University, Houston, TX, USA*

For a variety of quantum photonics applications, an ideal material system is being sought for stably producing high-purity single photons at a desired wavelength at room temperature. Recently, it has been demonstrated that individual single-wall carbon nanotubes (CNTs) with certain defects are promising room-temperature single-photon emitters with tube-diameter-dependent tunable near-infrared wavelengths. In this work, we investigate different ways to prepare CNT quantum emitters using chirality-enriched, functionalized, and suspended CNTs. The ultimate goal is to create a macroscopically ordered assembly of CNTs containing identical quantum defects with enhanced intensity and polarization stability through cooperative emission. Preparing such samples is challenging due to many factors such as difficulty of defect site isolation, cross talks between CNTs, anti-correlation errors and reduced collection efficiency of the emitted photons. To overcome these challenges, we are currently exploring two specific aligned-film fabrication processes: vacuum filtration and baked shear stress. In parallel to sample preparation, we perform atomic force microscopy, scanning electron microscopy, and Raman spectroscopy to locate and test the alignment of isolated CNTs and quantum defects on a substrate. Moreover, we are testing various sample architectures and assemblies to enhance the collection efficiency of photoluminescence signals, such as 1) coating the substrate with a gold thin film and 2) sandwiching the CNT layer with PMMA and surfactants, to protect tubes from their microenvironment and minimize any optical damages.

ECE-10 – Colossal Terahertz Magnetoresistance in $La_{1-x}Sr_xMnO_3$ Thin Films in High Magnetic Fields

Zhengyi Lu,[1,2] Fuyang Tay,[2,3] Andrey Baydin,[2,4] Paul Christenson,[5] Ethan Smith,[5] Jacob Thiele,[5] Maitri Warusawithana,[5] and Junichiro Kono[1,2,4,6]

[1]*Department of Physics, Rice University, Houston, Texas, USA.*
[2]Department of Electrical and Computer Engineering, Rice University, Houston, Texas 77005, USA.
[3]Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, Houston, Texas, 77005, USA.
[4]*Smalley-Curl Institute, Rice University, Houston, Texas, 77005, USA.*
[5]*Department of Physics, University of North Florida, Jacksonville, Florida, 32224, USA*
[6]Department of Materials Science and Nanoengineering, Rice University, Houston, Texas 77005, USA.

Lanthanum strontium manganite ($La_{1-x}Sr_xMnO_3$ or LSMO) exhibits a variety of exotic phases arising from complex competitions among the charge, spin, orbital, and lattice degrees of freedom, displaying various emergent phenomena as a function of x, temperature, and magnetic field. Furthermore, LSMO is promising for device applications as it shows colossal magnetoresistance (CMR), i.e., an enormous resistance change induced by an external magnetic field. However, due to the complicated many-body interactions, a microscopic theoretical understanding is still lacking for the various phase transitions and the unusual CMR effect in LSMO. Terahertz time-domain spectroscopy (THz-TDS) is an indispensable tool for providing novel insights into complex systems because it allows one to access low-energy collective excitations and probe the nature of charge carriers in materials. In this study, by using THz-TDS, we have determined the complex optical conductivity of $La_{0.7}Sr_{0.3}MnO_3$ and $La_{0.83}Sr_{0.17}MnO_3$ thin films in the THz frequency range in pulsed magnetic fields up to 25 T. The fields were produced by the Rice Advanced Magnet with Broadband Optics or RAMBO. The LSMO films were deposited on lanthanum aluminate substrates through molecular-beam epitaxy. Our results demonstrate the CMR effect in the THz range in both LSMO films at room temperature. Interestingly, the CMR effect generates a magnetoconductivity of 325% at 25 T and did not saturate. These results not only provide unique insights into the underlying mechanism behind the CMR effect but also shed light on the future fabrication of LSMO heterostructures that can eventually lead to the practical application of CMR in electronic devices.

ECE-11 – Developing a tailed primer assay using recombinase polymerase amplification for HPV 16 detection in low-resource settings

Ariel Ma,[1] Megan Chang,[1] and Rebecca Richards-Kortum[1]

[1]*Bioengineering, Rice University, Houston, TX, USA*

Cervical cancer is the fourth most commonly diagnosed cancer in women and is disproportionately prevalent in low- and middle-income countries (LMICs). Human papillomavirus (HPV) is the most common cause of cervical cancer, and thus, screening for the thirteen high-risk HPV (hrHPV) types is frequently used as a diagnostic standard (Hull, 2020). However, hrHPV detection often relies on polymerase chain reaction (PCR), which requires highly trained users and equipment that are typically unavailable in LMICs (Field, 2017). Recombinase polymerase amplification (RPA) is a sensitive DNA amplification method that operates at temperatures between 37-42°C in 20 minutes and requires little sample preparation and user skill, making it a promising alternative to PCR for simple, economical, and reliable rapid-testing in LMICs (Lobato, 2017). Results can be read on lateral flow assays (LFA), which further simplify instrumentation requirements and reduce cost. To detect HPV 16, the most oncogenic hrHPV type, RPA tailed primers that bind to HPV 16 oncogene E7 were generated by MATLAB. The tailed primers contain a non-specific sequence at the 5' terminus of the primer. The reverse complement of the tail is used to capture and visualize amplification products on an LFA. HPV 16 DNA, off-target HPV 52 DNA, and human genomic DNA were input into RPA with the experimental primer combinations. The products were subsequently amplified with qPCR or visualized on LFAs to identify sensitive and specific amplifications of products. An optimized tailed primer assay was determined for further optimization and validation in a multiplexed hrHPV test.

ECE-12 – Time lapses of urban surface temperatures using remote sensing

Anik Mandal,[1] Yuhao Liu,[1] and Ashok Veeraraghavan[2]

[1]*Electrical and Computer Engineering, RICE, Houston, TX, USA*

Land surface temperature (LST) is one of the key parameters in the physics of land surface processes from local through global scales. With the development of remote sensing from space, satellite data offers the possibility for measuring LST over the entire globe with sufficiently high temporal resolution and with spatially averaged values rather than point values. However, we cannot measure LST from satellite data in the regions of cloud cover because clouds block the transmission of thermal radiance and introduce scattering. In our work, we analyze the cloud cover over the top 20 US cities for the past four years (2018-2021) and study the correlations of LST with cloud cover. We show that there exists a correlation between the LST of a city, average cloud cover, and the annual precipitation rate. According to the data obtained, cities with higher average temperatures tend to have lower cloud cover, and vice versa. Also, cities that have higher cloud cover percentages are associated with higher annual precipitation rates. We conclude that different cities have different distributions of cloud cover. Therefore, we may need different sets of parameters to handle the removal of cloud coverage in LST maps for different cities in our subsequent studies.

ECE-13 – Analysis of the Implementation of Neural Networks using the FINN Framework

Emily Namm, Joseph Cavallaro

Department of Electrical and Computer Engineering, Rice University, Houston, TX, USA

Neural network solutions are becoming increasingly more popular in IOT applications. Many of these applications involve edge computation, in which the network is implemented on a small device with power and resource limitations. However, manually optimizing the network on an FPGA fabric in order to meet these constraints requires time and knowledge of lower-level design that not all software engineers possess. In this study we explore using FINN, an experimental tool for creating FPGA architectures from PyTorch models, as a possible method of quickly creating design prototypes. Although research has been done into the comparative accuracy and throughput of FINN designs, there is little to none involving power or resource use. To address this gap in the knowledge, we put a neural network designed for edge outlier detection through the FINN workflow onto a Xilinx Pynq-Z1 board, and compare the resulting overlay and its efficiency to one designed and optimized by hand, with emphasis on the relative power and resource consumption. If the FINN framework creates a comparable output, it offers a viable alternative that could be used to automate and expedite the design process.

ECE-14 – SAMReID: Siamese Network for Domain-Adaptive Memory-Based Person Re-ID

Bill Nguyen,[1*] Alma Torres,[1*] Kevin Ni,[1*] Taeho Choe,[1*] Shubha Hegde,[1*] Bryant Huang,[1*] and Joe Young[1*]

[1]*Electrical and Computer Engineering, Rice University, Houston, TX, USA*

Person identification (ID), is a vital component of surveillance, security, and human-robot interaction (HRI) applications. However, since robust person ID usually uses biometrics, which require subject cooperation, it is very inconvenient to use. Instead of verifying the subject's known identity, person re-identification (re-ID), a popular adjacent field, aims to match the identities of people who appear on multiple camera views, and has the advantage of operating on low-resolution images of subjects, which can be taken without direct cooperation. Re-ID approaches so far have either been image-based or gait-based, which struggle with cross-domain generalization and delivering enough identifying information respectively. Our SAMReID, an efficient general-purpose person ID system that derives intuition from re-ID, combines the gait approach's ability to adapt across domains with identifying information from the image-based approach. We pre-train a Siamese Resnet50 model on silhouette data and periodically fine-tune it with domain-specific color images during use, enabling constant re-adaptation to the target domain. The latent representation of each identity is stored in a KDTree-based memory, which is updated via moving average. We evaluate our system on the Duke and Market Re-ID datasets and show an improvement over standard Resnet, as well as real-time capability on a laptop GPU. To demonstrate the system's efficacy in the fields of surveillance and HRI, we implement it on an autonomous drone that reports and updates unique people's locations on a 3D-reconstructed map of the environment.

*These authors contributed equally to this work and share first authorship

ECE-15 – Determining Mental Model of Agent Playing the Prisoners Dilemma

Jessica Opsahl-Ong,[1] Itzel Olivos Castillo,[1] and Xaq Pitkow[2]

[1]*Computer Science, Rice University, Houston, TX, USA*
[2]*Electrical and Computer Engineering, Rice University, Houston, TX, USA*

A guiding question within the field of Neuroscience is how the brain's model of the world informs what actions it chooses to make. This internal model can be inferred from an observer's standpoint by parameterizing different mental models and finding the one with the highest probability of eliciting the observed actions. To test this technique, we can reformulate a "brain" as a rational computer agent and control for its internal model. This has been done in a single-agent context, and this summer we established a foundation to extend this research into a multi-agent setting. We chose the Prisoner's Dilemma as the setting, where the internal model of an agent playing the game can be characterized by a belief over their opponent's actions.

To begin this research, we focused on determining the mental model of a single rational agent. We accomplished this by optimizing agents against select iterated, discrete strategies established for playing the Prisoner's Dilemma. Each strategy can be represented as a Markov Decision Process (MDP), meaning we can solve for the optimal policy using a value-iteration algorithm. The policies optimized against a single strategy then play against players they were not optimized against. In this setting, we introduce observer, who must determine which strategy the policy thinks it's playing against by only using current and prior observations. Establishing the foundations of this research will allow future research to expand to a truly multi-agent setting, in which both agents are fully rational with respect to their mental model of the world.

ECE-16 – Novel Thermal Emitter for Increased TPV Efficiency

Samuel C Raphaelson[1], Ciril Samuel Prasad[2], Gururaj V. Naik[2]

[1]*Material Science and NanoEngineering, Rice University, Houston, TX, US*
[2]*Department of Electrical and Computer Engineering, Rice University, Houston, TX, US*

Thermophotovoltaic systems convert heat into electricity, enabling efficient waste heat recovery, long-term energy storage and long-distance energy transfer; however, current maximum conversion efficiency is limited [1]. Thermovoltaic systems consist of a heat source to provide energy, an emitter to convert the heat energy into thermal light, and photovoltaic cells to capture the emitted photons and generate electricity. This poster covers the process by which we determine the experimental efficiency of our novel emitter [2]. We have successfully simulated the maximum efficiency of the emitter as well as fabricated a sample emitter and characterized a compatible GaSb PV cell. We characterize the subsystems of our TPV for their efficiency and demonstrate the role of our novel emitter in improving the performance of the system.

[1] Omair et al. In: *Proceedings of the National Academy of Sciences*. 116.31. (2019), p. 15356
[2] Hassan S, Doiron CF, Naik GV. *Appl Phys Lett*. 116.023903. (2020), p.

ECE-17 – Generating OAM Beam using Massive MIMO platform

John Reko[1], Dr. Chia-Yi Yeh[1], Dr. Edward Knightly[1] *1*

Department of Electrical and Computer Engineering, Rice University

In an effort to increase wireless communication data rates, new EM wave characteristics need to be investigated. One of these characteristics is orbital angular momentum(OAM). There are many methods to generate beams with different OAM modes, but they require highly specialized systems that rely on different hardware to generate the beam. In an effort to minimize the hardware requirements, we designed a system that generates OAM beams using an existing MIMO platform. Using the RENEW platform at Rice University, we aimed to build a uniform circular array antenna (UCAA) transmitter and receiver. Multiple antenna mounting boards of different size and precision were manufactured in order to mount sixteen antennas for the UCAA transmitter and receiver. Then we conducted MATLAB simulations of the beam intensity and phase to estimate the behavior of antenna arrays of different shape, frequency, and OAM modes. Given the nature of the RENEW platform, the transmitter and receiver antennas need to be calibrated in order to deliver an accurate OAM mode. We developed a MATLAB script and python driver to calibrate the transmitter antennas using a long training sequence(LTS) and generate the data that would be modulated to create an OAM mode. There are issues involving carrier offset frequency for the transmitter calibration. The future of this project involves fixing those issues, applying a similar calibration process to the receiver antennas, and applying the calibration, mounting boards, and data generation to transmit data using an OAM beam.

ECE-18 – 3DML: Energy Efficient FPGA-based DNN in Xilinx FINN

Justin So and Joseph Cavallaro

Electrical and Computer Engineering, Rice University, Houston, Texas, USA

Given the rapid advancement of wireless technology, large amounts of time-vary data are produced and continuously simultaneously fed into the cloud. As the complexity of the networks increases, management and optimization for these networks are essential to increase the performance envisioned by next-generation networks. Our work proposes using machine learning-based solutions, namely one that uses an FPGA-based DNN (Deep Neural Network) written in Pytorch running in the Xilinx FINN environment, which can produce an energy-efficient algorithm fit for the growing complexity of wireless networks. The produced model should enable the data to be processed faster as the amount of redundant data is minimized over time.

ECE-19 – Understanding Channel State Information in Wireless Communication

Kenan Stredic, Oscar Benejaro, Andrew Sedlmayr, Ashutosh Sabharwal

Electrical and Computer Engineering, Rice University, Houston, Texas, USA
RENEW Project, Houston, Texas, USA

The Reconfigurable Ecosystem for Next-generation End-to-end Wireless project, also known as the RENEW project, at Rice University provides an open-source massive MIMO platform for research in wireless networking. The RENEWLab, a program that offers researchers methods for channel characterization, waveform evaluation, and creating datasets for machine learning, is one of the software frameworks utilized in the RENEW project. We run this on a Linux-based host machine using the SoapySDR software, an open-source generalized API and runtime library for interfacing with SDR devices, to communicate with the Iris Software Defined Radio hardware used in the wireless experiments. RENEWLab uses the C++-based framework Sounder, a python-based collection of analysis tools, and a Matlab-based collection of scripts to collect, record, and read the channel state information CSI obtained from the radios. The CSI is a mathematical characterization of a signal's effects when it travels from a transmitter to a receiver. The overarching objective we are trying to achieve from this research is to develop a tool that will visually and statistically fit different probability distributions to this channel data. We accomplish this by plotting histograms from the channel data, choosing a specific distribution to overlay on top of this data, and running a statistical test on which distribution is the best fit for the dataset. In the future, this research will increase the efficiency of the RENEWLab program by providing a simplified method for interpreting CSI datasets collected from radios.

ECE-20 – Flexible Probe for Time-of-Flight Transabdominal Fetal Pulse Oximetry

Sarah Go[1], Ankit Raghuram[2], Zijing Guo[2], Ashok Veeraraghavan[2]

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

Currently, physicians use the heart rate of a fetus to detect fetal distress and evaluate the need for an emergency Cesarean section. However, this method has a high rate of false positives. Fetal oxygenation levels (SpO2) are a more accurate metric, but the inaccessibility of the fetus prior to delivery prevents use of existing fingertip pulse oximetry technology. To address this gap, we are developing a time-of-flight near infrared spectroscopy (ToF-NIRS) based transabdominal fetal pulse oximetry system that can non-invasively measure fetal SpO2 during pregnancy, through a probe placed on the maternal abdomen. In this work, a probe for our system has been designed, prototyped and tested experimentally. The probe is made of flexible black silicone and secured with an adjustable elastic strap. Our probe design enables the high-density, variable arrangement of source and detector optical fibers and ensures good contact between the fibers and skin. Additionally, the probe is fabricated using a one-piece, reusable 3D-printed mold, reducing the fabrication time and facilitating future design modifications in comparison to other silicone molding methods. A potential design improvement was identified following experimental testing, whereby detectors are not arranged linearly but along circular arcs centered at the source. This enables combining of detected signals at the same radius to potentially improve the signal-to-noise ratio, which was verified using simulations and will be investigated experimentally. Overall, this research has produced a probe design that facilitates collection of optical data for ToF-NIRS measurements, while elucidating a fabrication method that enables fast prototyping and is amenable to future design modifications.

ECE-21 – Detection of Affect in Opioid Addicts

Natalie Finley, Zachary King, and Akane Sano

Electrical and Computer Engineering, Rice University, Houston, Texas, U.S.A.

Timely interventions are essential for optimal outcomes for opioid addiction disorders. Currently there are no tools to detect or predict opportunities for intervention because we cannot effectively detect drug cravings. Before detection is possible, it is necessary to predict affect in opioid addicts using data collected outside of a controlled laboratory setting. This study aims to build a machine learning model that can relate physiological, emotional, and contextual data in recently recovered opioid addicts to predict affect and subsequent drug cravings. Fitbits collect physiological data, four Ecological Momentary Assessments (EMAs) per day collect emotional data, and a phone application that tracks location and text messages collects contextual data. Physiological and contextual data collected within thirty minutes of the EMAs are used to train a semi-supervised multi-label classification model to relate stress and the type and intensity of three other self-reported emotions. There were significant limitations in data collection. The participants were noncompliant and completed on average less than two EMAs per day instead of four. Fewer than 1,000 datapoints were collected rather than the anticipated 8,000. Given the magnitude of the missing data, our model can only be used with limited application. Assessment of the accuracy of our model is still ongoing. To build more accurate models for these subjects in the future, experiment designs will need to account for data collection barriers, as it is likely that it will continue to be inconsistent.

ECE-22 – Diffusion Networks for Tensor Decomposition

Charan Santhirasegaran, Vishwanath Saragadam

Electrical and Computer Engineering, Rice University, Houston, TX, United States

Tensor decomposition – generating low-rank factors of a larger tensor – is crucial in a wide variety of applications including CT reconstruction, medical image denoising, classification, and video compressive sensing. A major problem with tensor decomposition is that available tools are not easily generalizable to different noise distributions. When non-Gaussian noise is introduced, current solutions such as PCA/SVD and nonnegative matrix factorization (NMF) are not optimal. Additionally, solutions for non-Gaussian noise require application-specific regularizers that are hard to compute. A major strength of diffusion networks is their strong generative prior, which implicitly removes the need for application-specific regularizers and therefore makes the network robust to non-Gaussian noise distributions. Additionally, computational tractability and robustness to low SNRs along with flexibility and sample quality make the diffusion network a very powerful tool for tensor decomposition.

ECE-23 – The Benefits of the Containerization of Real-Time Massive MIMO Baseband Processing using Docker

Noah Elzner,[1] Andrew Sedlmayer,[1] Oscar Bejarano[1], and Ashutosh Sabharwal[1]

[1]*Electrical and Computer Engineering, Rice University, Houston, TX, USA*

A Docker container is a standard unit of software which runs independently of its environment as the container holds all the code and the dependencies needed. By containerizing software with Docker, the encapsulation allows for application portability and for the containers to be lightweight, thus being more efficient with the resources available. Agora is a complete software realization of real-time massive MIMO baseband processing. Docker containers can communicate to each other locally on the same machine through usage of a Docker network, or they can also communicate to containers on different machines by a technique involving exposing ports on the container and syncing them to the machine. By containerizing the different parts of Agora and utilizing container to container communication, the processing can be distributed to different containers on separate servers, thus saving resources and allowing for more control on who can run Agora and where.

Nano-1 – Finding the Fluorescence Mechanism of Carbon Nanodots

Michelle Ahrens[1], Eric Gomez[1], and Stephan Link[1]

[1]Link Lab, Rice University, Houston, Texas, 77005, United States

Carbon nanodots, which are carbon nanostructures 10 nm or less in length, are being researched for their extensive applications in areas such as medicine, optoelectronics, and biosensing. They have adavantages compared to traditional quantum dots in terms of low cost, luminescence, and biocompatibility. However, a major obstacle to their commercial use is the disputed theories regarding the carbon dots' fluorescence mechanism. If we can distinguish diffraction limited individual carbon dots from carbon dot clusters at the nano level, we could determine how our single dots emit light. Here we tried to find photon traces and spectral information in an epifluorescent geometry; single particle fluorescence spectroscopy at 488 nm were done to resolve differences and heterogeneity at the nano level. The resulting raw data with traces was fitted onto a Lorentzian and parameters were extracted. Some conclusions can be drawn. We can use the photon traces and spectrscopy to see and distinguish single carbon dots from the aggregates. The presence of multiple peaks in the spectra and a gradual fall in the photon traces is a sign of aggregation. However, a spectra with two peaks, a larger and smaller one, is also not unusual amongst single carbon dots. Distinguishing between single dots and aggregates allows us to detect a blinking mechanism amongst single dots to extract information about the fluorescence mechanism.

Nano-2 – The Effects of Asphaltenes Onset Point of Precipitation on Water-in-Oil Emulsion Stability

Sharifa Akbary,[1] Nataira M. Pagán-Pagán,[2] and Dr. Amanda B. Marciel[2]

[1]*R-STEM Nano REU, Rice University, Houston, Texas, United States*
[2]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas, United States*

Asphaltenes represent the most polar, aromatic, and heaviest fraction of crude oil. Due to their heterogeneity in chemical composition, structure, and molecular weight, asphaltenes are defined by their solubility class. Therefore, asphaltenes are soluble in aromatic solvents such as toluene, and precipitate upon the addition of *n*-alkanes such as *n*-heptane or *n*-pentane. They are known to strongly adsorb at oil-water interfaces forming viscoelastic films that stabilize water-in-oil (W/O) emulsions. Besides, asphaltene forms aggregates and precipitates which leads to flow assurance problems. Therefore, it remains challenging to understand how the precipitation of asphaltenes influences the stability of (W/O) emulsions. To address this challenge, the model molecule Violanthrone-79 (VO-79) was used to investigate the onset point of precipitation. The onset point of precipitation, which is defined as the minimum amount of precipitant (e.g. *n*-heptane) it takes to precipitate the asphaltenes, was determined following the indirect method and UV-Vis spectroscopy. The experimental results showed that VO-79 precipitated, and the onset point of precipitation was observed at 30% vol. *n*-heptane. Studies on finding the relationship between the onset point of precipitation and emulsion stability will be further conducted by using microfluidic devices.

Nano-3 – Chemical Modification of Boron Nitride Nanotubes: Improving Dispersibility Using Aliphatic Amines Under Vilsmeier Conditions

Alma Gallardo Campa,[1] Michelle Duran Chaves,[2] and Matteo Pasquali[2]

[1]*R-STEM Nano REU, Rice University, Houston, Texas, USA*
[2]*Department of Chemical & Biomolecular Engineering, Department of Chemistry, Rice University, Houston, Texas 77005, United States*

The goal of this research project is to improve the dispersibility of boron nitride nanotubes (BNNTs) and create high concentration solutions of this material. Boron nitride nanotubes are a nanomaterial with a wide variety of potential electronic, mechanical, and biomedical applications due to their unique combination of properties. However, these properties are yet to be observed in their macroscopic state as desired. One of the main challenges of BNNT processing is the limited dispersibility that the material presents in organic and inorganic solvents due to its inertness. Here, we propose the functionalization of BNNTs with aliphatic amines. This study focuses on the chemical modification of boron nitride nanotubes by creating covalent bonds between the aliphatic amines and the BNNT walls under Vilsmeier conditions. The Vilsmeier reagent is a well-known salt consisting on N,N-dimethyliminium cation and chloride anion. The cation corresponds to the reactive component of interest that facilitates the bonding of the amines to the nanotubes. The covalent bonding between the aliphatic amines and the BNNTs is confirmed by infrared spectroscopy, thermogravimetric analysis, and X-ray photoelectron spectroscopy. The improved dispersibility of BNNTs in organic and inorganic solvents can make it more feasible to produce functional macroscopic materials. The results of the functionalization pose formidable applications to maintain the unique chemical properties of BNNTs in their macroscopic state.

Nano-4 – Developing Methods for the Analysis of in-situ 2D Crystal Growth

Cindy Huynh,[1] Andrew Hitt,[2] and Ming Tang[2]

[1]*R-STEM Nano REU, Rice University, Houston, Texas, United States*

[2]*Department of Material Science and NanoEngineering, Rice University, Houston, TX, USA*

CVD (Chemical Vapor Deposition) serves as the most appropriate method for creating MoS_2 (molybdenum disulfide) 2D crystals, which can be used for various applications in microelectronics. However, researchers are unable to conclude which experimental parameters would best influence the growth of MoS_2 2D crystals that would be well-suited for its applications. Unfortunately, a lack of analytical methods exists in terms of in-situ 2D crystal growth. This means researchers are not able to thoroughly analyze the effects in which certain parameters may have on the growth of 2D crystals. In this project, the fundamentals of Python, data science, and machine learning are applied to develop methods of analysis for in-situ 2D crystal growth. Within this project, a Python script simulating the growth of 2D crystals is used to generate images of 2D crystal clusters. These images are then used to train neural networks to interpret and count the number of 2D crystals within an image. Once the neural networks are able to count the number of simulated 2D crystals with sufficient accuracy, we can use the neural networks to assist the analysis of 2D MoS_2 crystalline growth within an experimental setting.

Nano-5 – Selectively Targeting Pathogenic RNA for Trans-Splicing of Toxic Genes

Yves-Langston M. Mays, Maria Claudia Villegas Kcam , Kim Wai Mo and James Chappell

BioSciences, Rice University, Houston, TX, USA

The Global Research on Antimicrobial Resistance Project estimates that antimicrobial resistance was responsible for 1.2 million deaths across 204 countries in 2019, with children under five years old representing 20% of the deceased. Trans-splicing Ribozymes, when combined with a target RNA sequence and a gene sequence, provide the desired protein output of a desired gene. Using a trans-splicing ribozyme to directly target pathogenic RNA has the potential to become a novel method of creating antimicrobials to combat the current rise in antimicrobial resistance. In this study, we use the trans-splicing ribozyme to deliver the genes for MazF and Lon protease, respectively, as cellular toxins. We expect, upon delivery of the aforementioned genes, to observe cellular death in targeted pathogenic cells, while non-targeted, non-pathogenic cells in consortia continue to function normally.

Nano-6 – Oscillating Gadolinium Diode Device for Thermal Regulation

Alexa Reyes, Qing Zhu, Geoff Wehmeyer

Department of Mechanical Engineering, William Marsh Rice University, Houston, Tx

To determine whether a new method of regulating temperature would be functional, we constructed a device that oscillates and behaves like a diode and tested it against fluctuating temperatures. There are limited methods for temperature regulation. These methods include thermoelectric devices, electric heating, convection, and liquid coolants. Could this device regulate the temperature of a sample, such as a copper plate? The resources for the oscillations are ubiquitous, as they are induced by forces of gravity and magnetization. The shuttle, which manages the waste heat of the sample, contains gadolinium and is responsible for the oscillations. A temperature fluctuating Peltier is used for the heating and cooling of the sample. The thermal contact resistance between the surfaces of the sample and the periodical Peltier prevented exceptional results. However, a thermal paste was used to alleviate the resistance and improve the experiment. The device is oriented in a manner where the bottom side is 15°C and the top side fluctuates from 24°C to 52°C. The shuttle begins to oscillate at around 28°C, keeping the sample about 8°C cooler than the periodical Peltier during its highest temperature. We have discovered a unique technique for regulating temperature. This opens new opportunities for waste heat management systems while maintaining open-access resources.

Nano-7 – Characterizing the DNA Methylation Landscape of Blood Cell Lineages using Structural Learning

Jordyn Sibert[1], Wei-Hao Lee[1,2], Sunny Kim[1], and Dr. Vicky Yao[1*]

[1] *Department of Computer Science, Rice University, Houston, Texas, United States of America*
[2] *Systems, Synthetic, and Physical Biology Program, Rice University, Houston, Texas, United States of America*

Inspired by the advancement of technologies in sequencing and genomic measurements of the human genome, researchers have sought out computational methods to observe and characterize DNA methylation landscapes to study their biological functions. DNA methylation regulates gene expression by adding a methyl group to regions of cytosine and guanine nucleotides that have a phosphate bond (CpG sites) within the genomic sequence. Interestingly, while the DNA segments remain unchanged, methylation can alter the activity of a DNA segment. Since this epigenetic process is linked to various biological functions such as cell differentiation, embryonic development, and variations in methylation have been observed in several diseases, it is crucial to create a way to better understand these relations. Previous research in this area has been limited to traditional machine learning (ML) models, where researchers have only been able to predict singular results. The novelty of our method lies in the addition of structural ML methods, which will enable multi-label classifications. Since blood cell lineages are clearly defined, we believe we can recapitulate these lineage ties with structured ML to establish a baseline that can later be expanded to more complex cells and tissue types. To begin this process, we have taken methylation datasets derived from a vast number of DNA methylation microarray data, and applied ML methods for baseline performance, and will additionally incorporate structural ML to integrate blood cell lineage information. In doing so, we aim to achieve better cell type predictions so that we can identify and investigate these informative features, such as methylation sites and their relating biological functions.

Nano-8 – Measuring Charge Transfer Through Plasmon Linewidth Broadening

Miley Wagner, Sadie Brasel, and Stephan Link

Department of Chemistry, Rice University, Houston, Texas, United States

Plasmon-induced charge transfer of single metal-semiconductor heterostructures can significantly improve the quality of photocatalysis and photovoltaics to build more efficient and longer lasting devices. Direct charge transfer has higher efficiencies than the conventional sequential mechanism as it is a decay pathway of the plasmon and therefore does not compete with cooling processes inside the metal. This property of direct charge transfer allows us to monitor it in the frequency domain as plasmon linewidth is inversely proportional to plasmon decay time. To measure direct charge transfer, single-particle dark-field spectroscopy is performed on a home-built microscope programmed with automatic focus abilities to gain spectra and measure the particles' peak wavelength. We compared TiO_2 and SiO_2 coated gold nanorod spectra and calculated direct charge transfer by subtracting bulk and radiation damping contributions from the plasmon linewidth. SiO_2 serves as the control since no charge transfer occurs in the non conducting medium. After analyses we have found that TiO_2 coated nanorods have larger charge transfer efficiencies than SiO_2 coated nanorod. Our work provides evidence of direct charge transfer and quantifies its efficiency in metal-semiconductor heterostructures, which is an essential step in utilizing charge transfer for the advancement of plasmon enhanced devices.

Nano-9 – Organization of confined colloidal chains in magnetic fields

Noelia Valdiveso,[1] Aldo Spatafora-Salazar,[1] and Sibani Lisa Biswal[1]

[1]*Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, USA*

This explorative study examines the organizational patterns and structures of clusters of colloidal chains under confined environments and external magnetic fields. Samples were prepared by confining the chains inside water droplets. This technique required stabilizing the water in mineral oil emulsion using surfactants. The emulsion was stabilized with the concentration levels of surfactants at 0.2 CMC of SDS and 1% w/w Span80. We then applied static and time-varying magnetic fields to monitor how the chains arranged when they repelled and attracted each other. Our preliminary observations indicate that the chains organized in the center of the droplet and all chains were oriented the same direction. We also found that the more flexible chains bend following the shape of the droplet while trying to also be in the same direction of the other chains. Further exploration using image analysis will help us develop a deeper comprehension of the chains' structural patterns and their application for new materials.

NEWT-1 – Nanosilica-Based Porous Superhydrophilic Spray-On Coating for Condensation Mitigation

Christopher Avalos,[1] Abduallah Alsinan,[1] Rawand M. Rasheed,[1] & Daniel J. Preston[2]

[1]*Department of Mechanical Engineering, Rice University, Houston, Texas, United States*

Condensation buildup on overhead plumbing from steam generated in industrial kitchens is a common occurrence that leads to health and safety issues resulting from d ripping condensate. In this NEWT REU summer research project, we develop a porous, superhydrophilic spray-on coating to mitigate dripping of condensate from overhead plumbing in industrial kitchens. A mixture of nanosilica, solvent, and epoxy binder is used to generate the nanosilica-based porous coating. We developed an experimental testbed comprised of a chilled water loop passed through metal plumbing to experimentally determine condensate uptake rates of the nanosilica-based superhydrophilic coating. We aim to compare the condensate uptake results of our coating to results from state-of-the-art condensation management solutions. The testbed has the capability to measure the mass of condensate absorbed via mass measurements and via a heat transfer correlation using temperature measurements from embedded thermocouples. This work has implications for kitchen sanitation, fog capture, and water recovery from cooling towers.

NEWT-2 – Minimizing Silica Concentration in Geothermal Brine by the Addition of Silica Seeds

Hannah Copland,[1] Xiaochuan Huang,[2] and Dr. Qilin Li[2]

[1]*NEWT REU Program, Rice University, Houston, Texas, United States*
[2]*Department of Civil and Environmental Engineering, Rice University, Houston, Texas, United States*

This study investigates the most favorable conditions for silica extraction from synthetic geothermal brine as a pre-treatment for lithium extraction. Minimal levels of silica within geothermal brine will enhance the effectiveness of lithium extraction due to limited silica interference. Several trials were conducted to explore improved conditions for silica removal in synthetic brine while mirroring a naturally occurring range of temperature and pH. Each trial maintained the brine solution at ninety-five degrees celsius and stirred five hundred rotations per minute. Samples were diluted from the brine at predetermined time increments, then hydrochloric acid and ammonium molybdate were added to each sample. After agitation, each sample was settled for five minutes and the silica concentration was measured via UV spectrometry. Trials were performed with no seeds, one to five micrometer seeds, fifteen to forty micrometer seeds, and a synthetic brine without calcium to observe seed performance without calcium interference. As expected, the results revealed trials with silica seeds added to the brine lowered the concentration most effectively. Although both caused the silica concentration to decrease, the smallest seeds (one to five micrometers in diameter) were more effective in lowering the brine's silica concentration, this is expected to be due to their larger surface area. Although the silica concentration decreased in the trial with a raised pH, a lower pH must be met to mock the conditions of natural geothermal brine. Discovery of refined methods to extract silica from synthetic geothermal brine will allow for more effective future lithium extraction.

NEWT-3 – Reverse Osmosis Concentrate Treatment with Fujifilm's Salt-Free Electrodialysis Metathesis

Melanie Cossio, [1] Tayia Oddonetto, [1] Shane Walker [2]

[1]*NEWT REU Program, University of Texas at El Paso, El Paso, Texas, United States*
[2]*Center for Inland Desalination Systems, University of Texas at El Paso, El Paso, Texas, United States*

Electrodialysis metathesis (EDM) is an electrically driven process used for desalination that allows for high recovery and concentrate management. In an EDM membrane stack, the voltage is applied between a cathode and an anode, which then passes ions through ion-exchange membranes. Alternating anion, cation, monovalent anion, and monovalent cation exchange membranes create two separate concentrate streams and a single diluate (product) stream. Traditional EDM requires the addition of a substitution solution, typically sodium chloride, for a metathesis reaction. Through collaboration with Fujifilm, the salt-free EDM process was tested at the Bureau of Reclamation's Water Quality Improvement Center (WQIC) in Yuma, Arizona. The competition was organized in an effort to maximize the recovery of fresh water from inland brackish desalination. A mobile system was equipped with six EDM stacks, treating WQIC RO concentrate in batch mode, achieving greater than 75% salinity reduction. The system produced a calcium-rich concentrate and a sulfate-rich concentrate (both of which are highly soluble) and batch recoveries ranging from 70-90%.

NEWT-4 – Harnessing Conjugation Systems for Engineering Microbes and Promoting Bioremediation through the Spread of bphC Dioxygenase Activity

Katya Escalante,[1] Tessa Crosby[2], and Lauren Stadler[2], PhD

[1]*NEWT REU Program, Rice University, Houston, Texas, US*
[2]*Civil and Environmental Engineering, Rice University, Houston, Texas, US*

Polycyclic aromatic hydrocarbons (PAHs) are environmental pollutants originating from the incomplete combustion of nonrenewable resources. PAHs are hazardous towards human health due to their carcinogenic properties and have been found in soil, aquatic, and atmospheric matrices. Plasmids can be conjugated between distantly related bacteria in environmental microbial communities, readily modifying their genetic landscape There is a lack of research surrounding the sustainability of the bphC gene among bacterial populations, as plasmids engineering studies fail to maintain transconjugant organisms across generations. In an attempt to address the uncertainty surrounding which plasmid characteristics lead to (1) high conjugation frequencies, (2) reduced fitness burden, and (3) stable expression of a dioxygenase payload, we employed four plasmids varying in size, copy number, and conjugative machinery. Through the implementation of the bphC gene, a dioxygenase codon isolated from crude oil spill sites, synthetic communities were engineered with an improved ability to degrade a model PAH. Furthermore, we utilized multiple soil-dwelling recipient pools as potential hosts for our bphC-engineered vectors. Due to the fact that our engineered pUC19 vector maintains a high copy number for a relatively small plasmid, recipient bacteria engineered with bphC amended pUC19 will degrade our model PAH at rates higher than transconjugant counterparts. Future studies will seek to determine favorable selective pressures encouraging long-term plasmid maintenance despite fitness costs.

NEWT-5 – Particulate Filtration with Additively Manufactured Inertial Filters

John M. Lentz,[1] Rawand M. Rasheed,[2] & Daniel J. Preston[2]

[1] *NEWT REU Program, Rice University, Houston, Texas, United States*
[2] *Department of Mechanical Engineering, Rice University, Houston, Texas, United States*

Particulate-laden flows pose a significant challenge to the efficient and reliable design of mechanical systems. This work describes the capture and retention of particulates in multiplexed inertial coalescence filters composed of parallel helical pathways, designed to capture fine particulate streams (<10 µm) through inertial separation while maintaining a low-pressure drop (<100 Pa). Capture efficiencies for particulates with an average size of 6 µm were characterized for both dry and wetted filters under varying flow conditions. Experimental capture efficiency results were compared to model predictions where dry filters, routinely underperformed model predictions past a threshold filter inlet flow rate whereas wetted filters remained in good agreement with model predictions for all observed inlet flow rates. The increased capture efficiency of wetted filters is enabled by the additional capillary forces used to retain particulates in the helical flow paths. This saturated multiplexed inertial filtration approach could find use in Lunar dust (>40 µm) filtration for Lunar life-support systems and particulate matter control in industrial settings.

NEWT-6 – Enhanced PFOA Removal from Water by Modified Nanomaterials

Juan F. Lopez,[1] Sheng Yin,[2] and Dino Villagran[2]

[1]Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment (NEWT) REU Program, The University of Texas at El Paso, El Paso, Texas, USA
[2]Department of Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, Texas, USA

Per- and Polyfluoroalkyl substances (PFAS), also known as forever chemicals, are a group of man-made chemicals found in the environment due to the inadequate disposal of products containing them. Perfluorooctanoic acid (PFOA) is one of these PFAS that has been shown to be harmful to human health. Nanomaterials such as Metal-Organic Frameworks (MOFs, compounds based on a transition metal bonded to organic ligands) have shown great promise for the degradation of PFAS, including PFOA, in water treatment. In this work, we synthesized UiO-66, a zirconium-based MOF, and later on modified it with graphite-like material, based on boron to study the composition and capacities for electro- and photo-degradation. The materials were analyzed and characterized by UV-Vis, SEM, PXRD, FT-IR & BET. Modified UiO-66 electro-degradation will be conducted with carbon paper modified electrodes as the working electrode, mercury chloride as a reference electrode, and a platinum counter electrode. Electro-characterization techniques cyclic voltammetry (CV), bulk electrolysis & square wave voltammetry (SWV) will be performed in an aqueous solution of potassium chloride (KCl). Modified UiO-66 Photo-degradation will be executed under sunlight expecting the UV-Light as the energy source for the material to act as a photocatalyst, quartz-glassware will be used to prevent UV absorbance. Both resulting samples after experiments will be tested for PFOA concentration using GC-MS, expecting the degradation of PFOA into smaller compounds until full recovery of drinkable water.

NEWT-7 – Nitrate-Based Fertilizer Recovery for Lettuce Growth

Andrea Victoria Maya[1], Gabriel Cerrón-Calle[2], Sergi Garcia-Segura[2]

[1] *NEWT REU Program, Arizona State University, Tempe, Arizona, United States*
[2] *School of Sustainable Engineering and Built Environment, Arizona State University, Tempe, Arizona, United States*

Agriculture relies on fertilizers to increase food yield and ensure food security. Fertilizer run-off has increased nitrate concentration in surface and groundwater. Nitrate concentrations over maximum concentration levels of 10 mg-N L^{-1} poses serious human and environmental risks. An efficient reusable fertilizer system is required to reduce water contamination and recover resources like NH_3 as add-valued products from waste. This study evaluates the reuse of nitrogen species (*i.e.,* NO_3^-, NO_2^- and NH_3) recovered through electrocatalytic treatment of simulated agricultural run-off using earth-abundant electrodes. Efficient N-species recovery was evaluated from the growth of *lactuca sativa*. To benchmark the positive impact of electrochemically recovered resources, the lettuce growth was compared against plants grown with tap water and Nutrients CNS17. Leaves and roots length were measured after two weeks presenting for tap water a length of 7.1 cm, CNS17 8.1 cm, and for recovered solution (NO_3^-:NH_3 1:1) 9.5 cm. Effects of pH on N-species distribution were quantified and their impacts on lettuce growth evaluated from leaves and roots length. After one week, at pH 4 (NO_3^-:NH_3 1:1.25) an average length of 7.0 cm, at pH 7 (NO_3^-:NH_3 1:1.35) 9.8 cm, and at pH 10 (NO_3^-:NH_3 1:1.15) 9.9 cm long. These results suggest that pH impacts plant growth. These results show high competitiveness of electrochemically recovered nutrients that can surpass the results observed for commercial fertilizers. Further studies are ongoing and a hydroponics system is being built to evaluate long-term impacts on plant growth.

NEWT-8 – Electrothermal Membrane Distillation (EMD) For Treating Hypersaline Feedwater

Carlos Gomez*, Jorge Medellin*, Naomi Fuentes, Ibrahim Abdallah

Nanotechnology Enabled Water Treatment (NEWT), Rice University, Houston, TX, 77005 USA
Department of Civil and Environmental Engineering, Rice University, Houston, TX, 77005 USA

It is estimated that one-fourth of the world's population lacks access to safe, reliable drinking water. A promising solution for treating saline water is using Electrothermal Membrane Distillation (EMD). The EMD process is based on using thermal elements over a hydrophobic membrane. The thermal element is connected to a power supply. When a certain electric voltage is applied, the heating element generates Joule heat that is conducted to the adjacent feed water. The heated feedwater evaporates at the water-membrane interface and the generated clean water vapor transfers to the permeated side, leaving the untreated saltwater behind. A spiral wounded EMD reactor is designed, developed, and tested over a wide range of operating parameters. Experiments have been conducted using different configurations of EMD (Sweeping Gas EMD and Direct Contact EMD) and feed water salinity (10,000 – 100,000 mg/L of NaCl). The data showed a 99 % salt removal with a product water flux of up to 2 Kg/m at 5 kW/m^2. Furthermore, a preliminary techno-economic analysis (TEA) study has been conducted to highlight areas where future R&D is needed and to quantify the relationship between engineering choices and economic outcomes. Finally, controlled-corrosion experiments have been conducted to evaluate the integrity of the heating elements of the EMD (316 st st) under different power densities and feedwater salinities. The turbidity, mass losses, surface morphology, and rate of corrosion were identified. The corrosion results revealed that differential aeration cells and dissimilar-metal corrosion cells were the major contributors to corroding the EMD elements.

*Jorge and Carlos have equal contribution

NEWT-9 – Inhibition of *Pseudomonas aeruginosa* biofilm through UV irradiation with

Modified Side-Emitting Optical Fibers

David Smith,[1] Zhe Zhao[2] and Paul Westerhoff[2] [1]

NEWT REU Program, Arizona State University, Tempe, Arizona, United States
2School of Sustainable Engineering and The Built Environment, Arizona State University, Tempe, Arizona, United States

A biofilm is an extracellular matrix which encases microorganisms, allowing for attachment to surfaces and optimal survival conditions. Biofilms grow on nearly all surfaces in contact with water. Bacterial biofilms in potable water systems pose financial burden to water treatment plants and potential health threats (e.g. pathogenic bacteria) to the general public. For example, the causative agent in Legionnaires' disease, *Legionella pneumophila* is found in many biofilms. Existing biofilm treatment methods rely on chemical agents (i.e., chlorine), yet biofilm control is challenging because chlorine decays over time and with distance to its point of application. Germicidal ultraviolet (UV) radiation at 250 to 290 nm has shown antimicrobial properties against the formation of biofilms created by bacteria including *Pseudomonas aeruginosa.* The challenge has been how to deliver germicidal UV light in small diameter plumbing fixtures where biofilms grow. We investigate the effects of modification of side-emitting optical fibers (SEOFs) and irradiation time on UV performance to maximize the efficacy of UV radiation against a model bacterium, *Pseudomonas aeruginosa*. Our studies measure a zone of inhibition on surfaces caused by UV radiation delivered by flexible 0.5 mm diameter SEOFs. Using a facile method to rough the surface of the SEOFs, we demonstrate how this increases side emission of UV light, thus increasing the zone of inhibition. Our studies show that longer periods of irradiation lead to more biofilm control. These findings suggest that UV radiation, alongside modified optical fibers, is an effective and scalable method of inhibiting biofilm formation.

NEWT-10 – Solar-Assisted Direct Contact Membrane Distillation

Aislinn Varela[1,2], Mohamed E.A. Ali[2], Mohammed Bashammakh[2], François Perreault[1,2]

[1]*Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment Research Experience for Community College Students, Arizona State University, Tempe, AZ 85281*

[2]*Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment, School of Sustainable Engineering and the Built Environment, Arizona State University, Tempe, AZ 85281*

Direct contact membrane distillation (DCMD) is a thermally-driven process of water purification involving a microporous, hydrophobic membrane which allows water vapor from the feed to transport across the membrane to the permeate side while leaving dissolved solids behind. Reverse Osmosis (RO) is the leading method of water desalination globally, but the advantage of DCMD is its ability to utilize ambient low-grade heat sources to treat concentrated brine, especially from RO retentate. The management of RO brine is crucial for inland water desalination systems where underground injection and oceanic disposal are not feasible. The current challenge to membrane distillation addressed in this work is membrane fouling, which leads to a decline in membrane flux and requires frequent cleanings. Membrane surface coatings have been demonstrated to mitigate surface fouling by reducing temperature polarization. Using a Carbon Black composite with Polyinyl Alcohol coating applied over commercial 100 μm PTFE membranes with a pore diameter of 0.2 μm, a decrease in surface salt crystallization and reduction in flux decline were observed when placed under a solar simulator of 95 mW. Each membrane surface was characterized through contact angle measurement to quantify hydrophobicity and zeta potential measurement to quantify surface charge. Using a scanning electron microscope, photos of the membrane surfaces revealed a significant reduction in the size of salt crystals when compared to the uncoated membranes. The Carbon Black coated membranes had a breakpoint in the flux at a concentration factor of 3.5, while uncoated membranes experienced a degradation in their performance at 2-2.5.

HS-1 – A low-cost reusable probe holder for high resolution in-vivo imaging

Alex Schwarz[1], Jackson Coole[1], Rebecca Richards-Kortum[1]

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

Fiber optic fluorescence microscopes have been used to perform in vivo imaging of cell nuclei to detect dysplasia and cancer in a variety of anatomical sites. However, fiber optic probes can be difficult to hold steadily while acquiring images of tissue due to their small diameter (~1mm) and limited flexibility. Our lab has previously developed low-cost handheld probe holders that can be readily made using commercially available 3D printing systems. However, older variants of the probe holder were not disinfectable due to channels inside the holder. The necessary components for a successful probe holder that addresses these issues are: (1) a fully disinfectable probe holder, meaning that it has no interior channels that could potentially have organic material trapped inside; (2) the probe holder must be comfortable to hold and snugly hold the probe in place; and (3) the probe must be easily removable without excess force that may harm the probe. The probe holder does this by using squares with a slight overhang on alternating sides of the indent that runs vertically along the entire holder, which holds the probe tightly. The tip of the probe is held steady by rings at the distal end of the probe holder and/or a ligature attached to the distal tip. There are no moving parts in the holder, no assembly needed nor is there any complicated method of fastening the probe into the holder. Prototypes were modelled in NomadSculpt and printed on an Anycubic Photon resin 3D printer.