

#### Session G Abstracts

## Characterization of ${\rm TiO_2}$ electron transport layers for transition metal dichalcogenide photovoltaics

Belle L. Chen

Mentors: Harry A. Atwater, Jr., and Rachel Tham

Transition metal dichalcogenides (TMDs) are a class of 2D semiconductor materials that possess high optical absorption, passivated surfaces, and favorable mechanical and electrical properties that are well-suited for applications requiring light, flexible, and efficient solar cells. However, the highest performing TMD theoretical power conversion efficiencies expected of these materials, primarily due to recombination losses at the TMD and electrode interface. High efficiency solar cells with other photoactive semiconductors, such as silicon or perovskites, typically incorporate carrier-selective contacts, or transport layers. These layers facilitate the movement of the photogenerated charges from the photoactive layer to improve the device carrier collection and thereby increase the overall device efficiency. Here, we investigate TiO<sub>2</sub> as an electron transport layer due to its favorable band alignment and wide bandgap properties. TiO<sub>2</sub> films were deposited through atomic layer deposition atop numerous stack geometries and subjugated to a suite of post-processing conditions. Film quality and composition were verified through techniques such as Raman Spectroscopy, X-Ray Photoelectron Spectroscopy, and Atomic Force Microscopy. The TiO<sub>2</sub> optical constants were also measured with ellipsometry. Finally, the viability of the TiO<sub>2</sub> electron transport layer in a TMD solar cell was assessed.

#### Simulations of Shor's algorithm with reduced density matrices

Nathan Jay

Mentor: Marco Bernardi

Shor's algorithm is a quantum algorithm that provides superpolynomial speedup in factoring integers. Classical simulations of this algorithm require exponential resources, but using reduced density matrices provides a speedup. This project further explores using reduced density matrices in simulation of the core subroutine in Shor's algorithm—phase estimation. Through simulation of phase estimation circuits, pitfalls of 3–RDM simulations are found at the SWAP gates, as well as when tracing down to 1–RDMs. A more faithful SWAP treatment within the RDM picture is outlined, and efficient tracing procedures are identified as a key direction for improvement

#### Practical spaceplates for ultra-compact optical systems

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Mentors: Andrei Faraon and Phillippe M. Pearson

The miniaturization of optical systems has driven significant interest in flat optical elements that can replace bulky free-space propagation regions. Spaceplate optical metasurfaces offer a promising solution by replicating the phase accumulation of free-space propagation within a significantly thinner structure. However, existing spaceplate designs face significantly limiting trade-offs between compression ratio (R), numerical aperture (NA), bandwidth, and transmission efficiency, restricting their practical application. In this work, we leverage forward- and inverse-design techniques to engineer, fabricate, and experimentally demonstrate photonic crystal slab spaceplates with high performance across all key metrics. These designs are tailored for the mid-IR, yet readily adaptable to other wavelengths through appropriate material selection.

Initial designs were developed through manual parameter exploration and validated with RCWA and FDTD simulations, yielding practical structures on SiO2 and sapphire with simulated compression ratios up to R  $\approx$  70, an NA of 0.2, and acceptable transmittance over a 50 nm bandwidth. Inverse design techniques were leveraged to further optimize these geometries. The designs are now being

fabricated and experimentally characterized. To our knowledge, this work will constitute the first experimental demonstration of a photonic crystal slab spaceplate, paving the way for the development of ultra-compact optical systems in imaging and integrated photonics.

# Developing and optimizing an acousto-optic deflector (AOD) system for trapped-ion quantum logic operations

Mark A. Gherghetta

Mentors: Crystal Noel, Manuel A. Endres, and Jerry Chen

Trapped-ion quantum computing has proven to be a promising approach in achieving full-scale quantum computers. In this architecture, the qubit state is encoded in the electronic states of the ion. Single and two-qubit gate operations on this platform are realized with individually addressable laser pulses incident on a chain of ions. Multiple beams can be generated by radio-frequency (RF) driven diffraction through an AOD. Due to the small spacing of ions in a chain, any laser beam incident on a single ion will inevitably leak onto neighboring ions. This crosstalk error poses a challenge that hinders further scalability of the platform. Therefore, a method for minimizing crosstalk errors is desired. In this project, an experimental AOD system was developed to study potential error sources. Beam output was analyzed, and AOD RF input was optimized for amplitude configurability and minimization of crosstalk using a gradient-based optimization algorithm. This analysis is crucial for two-qubit entangling gates and multi-qubit gates used in sophisticated quantum simulations, which will be utilized in a future novel trapped-ion system.

### Mitigating decoherence in superconducting qubits via a floating merged-element transmon embedded in a phononic shield

Benjamin L. Boone

Mentors: Oskar J. Painter and Matthew Davidson

The development of long-lived superconducting qubits is challenged by decoherence due to both Two Level Systems (TLSs) in dielectric materials and quasiparticles in superconducting films. Current research in the Painter Lab focuses on the development of a new qubit design, a merged-element transmon (MET) embedded in a phononic shield, to minimize TLSs and maximize qubit lifetime. The effect of quasiparticle participation can also be reduced by removing the qubit's connection to the superconducting ground plane, a major reservoir for quasiparticle generation. This project investigates the design implications surrounding the creation of a floating qubit. We demonstrate the theoretical equivalence between a grounded and ungrounded MET and confirm it computationally. We analyze the relationship between the required qubit drive voltage and capacitance. We simulate the electrostatic and quantum-mechanical properties of the device to arrive at optimal geometries and drive based on our analysis. Findings indicate that a floating MET is both a feasible and reasonable implementation strategy for our novel qubit design.

#### Nanofabrication of metal-vacuum-metal tunnel junctions via angle deposition

Daniel Q. Wareham

Mentors: Axel Scherer and Geraldine Silva Galindo

Metal-Vacuum-Metal (MVM) diodes and triodes are a promising alternative to silicon-based Field Effect Transistors (FETs) which, for decades, have been the fundamental unit of electronics, but whose continued miniaturization now faces substantial technological hurdles. In MVM diodes (or junctions), electrons flow from an emitter to an anode either after field emission or via direct quantum tunnelling. Nearby third and fourth electrodes can be used to modulate this flow, making a transistor. In this project, we fabricated and characterised a MVM tunnel junction, doing so with a geometry which easily allows for the future creation of MVM triodes. Ytterbium(II) Fluoride, a novel inorganic self-developing e-beam resist allowing for future vacuum-only processing, was deposited on bulk silicon, onto which trenches of less than 10 nm in width were created. We then deposited metal at an angle toward the side of the trenches and stopped right before the two sides contact, leaving a 1-2 nm gap small enough to allow for tunnelling effects. We intend to confirm the success of forming an isolated junction with electron microscope voltage imaging and detect the presence of tunnelling when probing by measuring the linear I-V characteristic expected of MVM tunnel junctions.

#### Deterministic single atom loading into optical tweezers

Sanzhar Bissenali

Mentors: Jeff Thompson, Andrei Faraon, and Michael Peper

Neutral atom quantum computing is a promising platform for scalable quantum information processing. One of the key challenges in the field is achieving high-probability single-atom loading into optical tweezer traps. The current standard method—parity projection—has several drawbacks, including millisecond-scale time and limited efficiency. We propose an alternative, deterministic approach for atom loading that overcomes these limitations. By utilizing the rich electronic structure of <sup>171</sup>Yb and exploiting collective many-body Rabi oscillations, we computationally demonstrate that highly efficient single-atom loading is achievable, provided sufficient laser power and a long-lived Rydberg state.

### Design and implementation of a tunable piezoelectric pressure system for layered 2D materials

Richard H. Feng

Mentor: Stevan Nadj-Perge

Moiré materials are systems of layered two-dimensional (2D) materials. Given the freedom of materials to stack, one can compose devices with distinct physical and electronic characteristics. By exploiting the stacking and rotational degrees of freedom, these systems can exhibit novel phenomena such as superconductivity and unconventional magnetism. The application of high pressure to such systems is of recent interest to the 2D materials community, as pressure changes the coupling between the layers and alters the electronic structure. Currently, this pressure is applied using hydrostatic methods or diamond anvil cells, which are powerful but involve significant technological and experimental overhead. In this project, we are developing a new type of pressure cell that uses simple piezoelectric elements to apply tunable, in-situ force directly on the device. Our prototype is compact, compatible with cryogenic environments, and is expected to reach pressures comparable to other high-pressure techniques, with the added advantage of fine, real-time control.

#### Photoinduced Ag doping for stabilizing mixed-halide perovskites

Hana Hisamune

Mentors: Barry Rand, Harry A. Atwater, Jr., and Julia C. Brubach

Mixed-halide perovskites offer tunable bandgaps for tandem solar cells, which can exceed the maximum efficiency of single-junction solar cells by harnessing a broader range of the solar spectrum. However, their long-term stability is limited by halide oxidation and segregation under operational conditions, which can lead to permanent film degradation and reduced device performance. This project investigates photoinduced silver (Ag<sup>+</sup>) doping as a stabilization treatment to suppress halide segregation in mixed-halide perovskite films. Under illumination, Ag is expected to oxidize spontaneously and migrate into the perovskite lattice via iodine interstitial sites, thereby suppressing halide oxidation. Using photoluminescence (PL) spectroscopy, we tracked the spectral evolution of Agcoated films and observed a clear reduction in redshift associated with iodide-rich phase formation compared to untreated controls. We optimized this treatment by introducing a LiF wetting layer to improve Ag coverage, and systematically investigated different metal cappings and thicknesses to identify the most effective parameters for suppressing halide segregation. Furthermore, we performed X-ray photoelectron spectroscopy (XPS) to probe iodine–metal interactions to confirm the mechanism behind suppressed halide migration and to explain the variations in PL response observed across different metal treatments.

### Gradient-controlled and templated TBA-based freeze casting of porous prismatic SiOC scaffolds

Audrey S. Chyung

Mentors: Katherine T. Faber and Wesley D. Patel

Tert-butyl alcohol-based freeze-casting yields scaffolds with a prismatic pore morphology, which is highly permeable along the axis of pore orientation and not achieved using common freeze-casting solvents. However, tert-butyl alcohol's tendency to supercool leads to rapid, uncontrolled nucleation and crystal growth upon freezing. The resulting off-axis pore domains reduce bulk permeability. A double-sided, gradient-controlled freeze-casting setup is hypothesized to reduce supercooling and encourage growth in the direction of the imposed temperature gradient. A templated bottom surface may further reduce supercooling and control initial crystal nucleation to select for vertically-oriented grains. In the current research, we obtain a phase diagram of the tert-butyl alcoholpolymethylsiloxane system using differential scanning calorimetry to quantify the degree of supercooling occurring during freezing and better inform freezing profile design. We develop a gradient-controlled freezing profile and template. Image analysis techniques are used to measure freezing front velocity. Scanning electron microscopy and a variable-pressure fluid flow apparatus are used to evaluate pore morphology, pore alignment, and permeability. Mercury intrusion porosimetry is used to measure porosity and pore size distribution. Compressive strengths and permeabilities of prismatic, lamellar, and dendritic structures are measured to compare flow properties, energy input, and mechanical stability of the scaffolds for applications in filtration.

# Combining magnetic susceptibility measurements with a mathematical approach to modeling inductive coils to approximate the London penetration depths of superconductors Jonathan Dawit

Mentors: Joseph L. Falson and Reiley J. Dorrian

Two-dimensional quantum materials have been shown to exhibit a multitude of effects that are of great significance. Superconductance is one of the aforementioned properties that has applications in the fields of quantum computing, magnetic resonance imaging, and far more. However, to analyze the properties of these superconductors, one must find their London penetration depths, a measure of how deeply external magnetic fields penetrate the surface of superconductors. Here, we present a technique to measure the London penetration depth based on changes in the magnetic fields of three inductive coils through the Meissner effect. We created a 3D-printed mount for the superconducting sample, and created an adjacent rod with three inductive coils, which allows us to measure the changes in the magnetic field. We then analyze our findings with a Python program, made to convert these changes in the magnetic field to the London penetration depth.

#### A LEEM study on graphene growth

Yan Che

Mentors: Joseph L. Falson and Ivan S. Bespalov

The discovery of graphene, a one-atom-thick layer of carbon atoms, by Geim and Novoselov has triggered intense research on two-dimensional materials (2DM). Due to their exceptional properties, these materials hold great potential for applications in next-generation electronics. However, for practical use, a major requirement is the ability to synthesize individual 2DM islands on a devicecompatible scale. One promising approach for large-scale synthesis involves combining layer-by-layer growth with tools for in-situ monitoring of the growth process, allowing observation of 2D material formation at every stage. In the present research, we employ Molecular Beam Epitaxy (MBE) together with Low-Energy Electron Microscopy (LEEM), area-selected Low-Energy Electron Diffraction (μLEED), and LEEM I-V to study the growth and structure of graphene and graphene-based heterostructures, providing a unique platform for real-time, real-and reciprocal-space observation of 2DM at the devicerelevant scale. The growth and evolution of graphene islands were monitored by LEEM, while µLEED provided information about the atomic structure, and LEEM I-V yielded information about local workfunction variations. The controlled and scalable synthesis presented in this work enables exploration of large-scale graphene and graphene-based heterostructures growth, which, when performed on semiconducting substrates, can provide a usable platform for measuring 2D material transport properties.