Caltech
Student-Faculty Programs

Session I Abstracts

Control of surface morphology in spalled thin silicon for space solar power applications
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Mentors: Harry A. Atwater, Jr., Andy Nyholm, Elsie P. Loukiantchenko, and Elsie P. Loukiantchenko

Space solar power requires photovoltaic systems with high power-to-mass ratios, motivating thin silicon devices. Spalling offers a scalable, kerfless route to exfoliate thin layers of silicon substrate. Since Si is an indirect bandgap material, thinning reduces optical absorption of photons. However, controlled corrugations may enhance light trapping due to increased scattering. The effect of processing conditions on spall morphology remains poorly understood. We investigate the effects of wafer orientation, crack-propagation direction, and electroplating conditions using surface characterization tools and finite element analysis. Si(100) commonly develops crystallographic corrugations, while river lines occur in both Si(100) and Si(111) and intensify near lateral edges. A 3D FEA COMSOL model is built to connect this surface feature to an opposite-signed, edge-enhanced out-of-plane shear and mixed-mode I+III fracture. Directional studies indicate that Si(111) spalling along the ⟨110⟩ orientations generally produces smoother surfaces than along the ⟨211⟩ orientations, whileSi(100) results primarily reveal smooth, corrugation-free regions along the ⟨100⟩ orientations. Electroplating conditions remain ongoing work and are expected to reveal how stressor residual stress gives rise to distinct morphological features.

Surface plasmon resonance spectroscopy for investigating the growth of molecular additive layers on copper for CO_2 reduction
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Mentors: Harry A. Atwater, Jr. and Ellis Spickermann

The electrochemical CO_2 reduction reaction (CRR) utilizes renewable energy sources and stores energy longer than any typical battery or capacitor, and can be done safely and cheaply in aqueous solutions. However, in these solutions, the CRR suffers from the uncontrolled occurrence of the hydrogen evolution reaction (HER), lowering the efficiency of CO_2 reduction. Molecular additives, particularly *n*-tolyl-pyridinium, have been previously shown to suppress HER. We found that in electrochemical cells, *n*-tolyl-pyridinium was deposited on the cathode when a voltage of around -0.5 V vs SHE or lower was applied, with the deposition rate increasing at lower voltages. When running the cell while sparging with Ar, the current approached 0 due to the lack of CRR and suppression of HER as the additive layer grew. These final additive layers were determined to be around 100 nm thick using ellipsometry. *In-situ* surface plasmon resonance (SPR) spectroscopy was also used to investigate *n*-tolyl-pyridinium layer growth rates. The redshift of the layer's characteristic SPR dip was examined at different growth times, and the layer thicknesses were measured using ellipsometry. The final thickness could not be examined as the SPR dip redshifted out of the range of the spectrometer. The interim thickness points were instead used to model the layer growth in COMSOL based on the change in the SPR spectrum across the whole growth process.

SPR analysis indicated that a copper-water interface reappeared when lower voltages were applied. Prior to any applied voltage, the SPR spectrum of simple copper-electrolyte showed an SPR dip at around 570 nm. At an applied voltage of around -0.5V vs SHE the additive layer grows and the SPR dip redshifts past 900 nm, out of the range of the spectrometer. Regardless of the thickness of the additive deposited beforehand, at around -1.2 V vs SHE, an SPR dip at 575 nm appeared and the general shape of the spectrum became similar to that of a simple copper-water interface. Below -1.2 V, the SPR dip redshifted 10-20 nm. COMSOL modeling indicated that these results could be generated by the presence of a water layer which decreased in thickness as the voltage decreased. This water layer could be formed by the additive momentarily peeling off of the copper due to swelling or bubbling from gas production. This water layer disappeared once voltages were returned to above -1.2 V.

Utilizing these observations, we aim to control the thickness and growth rates of the *n*-tolyl-pyridinium layer in CO_2 reduction cells. We plan to control the final layer thickness by changing the concentration of *n*-tolyl-pyridinium in the electrolyte, and control the final growth rate by changing the applied voltage.

Developing a new optical spectrometer to investigate the timing of ionization transitions relative to other plasma phenomena in the Caltech jet experiment
Miguel G. Guerra Zeferino
Mentors: Paul M. Bellan and Joshua Q. Morgan

This project aims to finalize the development of a new, fast optical spectrometer and then use this to measure the time evolution of the emission spectrum from the plasma in the Bellan Plasma Group's jet experiment at Caltech. In the Caltech jet experiment, a jet of plasma is created which develops a series of instabilities and eventually breaks apart. When the jet breaks apart, a ubiquitous plasma phenomenon called magnetic reconnection occurs, where the magnetic field rapidly reorganizes and releases energy into the plasma. X-rays are observed at this time, which is unexpected since it requires electrons to reach greater energies than were initially believed to be possible. Using data obtained from the new spectrometer, the timing of key transitions in the emission spectrum in relation to the emission of X-rays will be investigated to provide a high-temporal-resolution diagnostic of the plasma around the time of magnetic reconnection, which may be used by the lead plasma physicists to develop models explaining the X-ray bursts.

On-chip mid-infrared optical parametric oscillation in thin-film lithium niobate-on-sapphire
Elizabeth Seward
Mentors: Alireza Marandi and Selina Zhou

Optical parametric oscillators (OPOs) based on second-order ($\chi^{(2)}$) nonlinear interactions provide a versatile route to coherent, widely tunable light at wavelengths inaccessible to direct laser gain media, making them a key tool for mid-infrared spectroscopy and sensing. While bulk and fiber-based OPOs have long served this role, their footprint, cost, and power requirements limit deployment outside the laboratory. The advent of thin-film lithium niobate (TFLN) nanophotonics, offering tight mode confinement and engineerable dispersion, has enabled chip-scale OPOs with dramatically reduced thresholds. However, on-chip OPOs have so far been largely confined to signal/idler pairs below [3.5~μm], falling short of the spectral reach of their bulk counterparts.

This work presents an on-chip, doubly resonant OPO fabricated on a TFLN-on-sapphire platform, pumped by a pulsed telecom laser near 1550~nm. Using periodically poled, dispersion-engineered waveguides, we demonstrate parametric oscillation with emission spanning from degeneracy to 4~μm. We characterize the device threshold behavior, measuring an oscillation threshold of 5.5 W on-chip pump peak power, and quantify cavity performance through finesse and free-spectral-range (FSR) measurements across the signal and idler resonances. On-chip signal and idler powers are calibrated using detector gain and filter transmission corrections, yielding a peak conversion efficiency of 0.4\%. Pump-wavelength tuning is shown to continuously shift the idler emission, consistent with the resonator's group-velocity-matched design.

These results establish a compact, low-threshold source of tunable mid-infrared light directly accessible from a telecom pump, and point toward integrated platforms for on-chip molecular spectroscopy and sensing applications.

First-principles approach to optical excitations of coherent phonons
Han Na Shin
Mentors: Marco Bernardi and Sergei Kliavinek

Recent experimental advances in nonlinear phononics have demonstrated the ability to induce and manipulate properties in materials via coherent phonon excitations. These results highlight the capabilities of engineering practical non-equilibrium functionalities for memory storage and integrated microelectronics, while also playing important roles in chemical and biological activity in molecular systems. However, a comprehensive framework capable of describing, simulating, and predicting the full electron-phonon system in this phenomenon is lacking. We aim to fill in this theoretical gap by developing a first-principles framework that combines the Boltzmann transport equation (BTE), which captures the thermal phonon population, and an equation of motion that encodes the presence of coherence via displacement amplitudes. This framework accounts for phonon-phonon and electron-phonon interactions, while explicitly retaining both coherent phonon and thermal phonon contributions. Further, we extend this approach to encompass spatiotemporal order arising from parametric resonance, providing a unified first-principles approach to coherent dynamics and their subsequent energy dissipation into thermal phonon and electron populations.

MACE-H-LR: Incorporating long-range interactions into equivariant Hamiltonian prediction
Jeremiah Bailey
Mentors: Marco Bernardi and Yao Luo

Accurate prediction of Hamiltonians is important for efficiently modeling the electronic properties of materials. Equivariant machine-learning models such as MACE-H can learn Hamiltonians from local atomic environments, but finite-cutoff architectures may have difficulty representing long-range interactions that extend beyond the local neighborhood. This work introduces MACE-H-LR, a physics-informed extension of MACE-H designed to predict the full Hamiltonian while explicitly accounting for both short-range and long-range contributions.

The short-range contribution is learned using an equivariant message-passing neural network, while the long-range component is incorporated through a separate physically motivated formulation based on the atomic structure and periodic simulation cell. The model predicts Hamiltonian matrix elements between atomic orbitals while preserving the rotational and geometric symmetries of the system. Developing the framework required consistent treatment of atomic-orbital indices, lattice translations, tensor dimensions, coordinate conventions, and periodic boundary conditions.

Following training, MACE-H-LR was evaluated on structures excluded from the training dataset and compared with the original short-range MACE-H model. The evaluation examined prediction errors, convergence behavior, and the relative influence of the short-range and long-range contributions. The results demonstrate the feasibility of combining equivariant machine learning with an explicit long-range treatment for full Hamiltonian prediction. This framework provides a foundation for more accurate and physically consistent electronic-structure models, particularly for materials in which nonlocal interactions significantly influence the Hamiltonian.

Localized reconstruction of electron–phonon interactions from first principles
Kehan Jiao
Mentors: Marco Bernardi and Yao Luo

This project develops a localized framework for reconstructing electron–phonon interactions from first-principles calculations. The central challenge is to retain the accuracy of a plane-wave description while obtaining a compact atomic-orbital representation that is easier to interpret and integrate into data-driven models. We first compare the reconstructed atomic-orbital band structure with the original plane-wave result to assess the fidelity of the electronic representation. We then use cross-validated learning curves to quantify how the accuracy of fitted Hamiltonian derivatives improves as additional displaced structures are included. As an independent validation of the nuclear-motion treatment, we reproduce the anharmonic phonon dispersion of palladium hydride using the stochastic self-consistent harmonic approximation. Finally, we compare the reconstructed electron–phonon coupling strengths associated with hydrogen–hydrogen, hydrogen–palladium, and palladium–palladium hopping channels and examine their temperature dependence. These results identify the local electronic processes most sensitive to atomic motion and establish a foundation for studying anharmonic and higher-order electron–phonon interactions, particularly electron–two-phonon coupling.

First-principles modeling of phonon-mediated anomalous Hall transport in magnetic materials
Chieh-An Yu
Mentors: Marco Bernardi and Lauren A. Tan

The anomalous Hall effect (AHE) is a fundamental transport phenomenon in magnetic materials, where an applied electric field generates a transverse voltage through the interplay between spin-orbit coupling, electronic band structure, and carrier scattering. While intrinsic AHE arising from Berry curvature and conventional extrinsic mechanisms caused by impurity scattering have been extensively studied, the influence of phonon-mediated scattering on anomalous Hall transport at finite temperature remains an open theoretical challenge.

In this project, we investigate anomalous Hall transport from both theoretical and first-principles perspectives. We develop a theoretical framework for phonon-mediated extrinsic AHE by deriving the contributions from skew scattering and side-jump mechanisms within the semiclassical Boltzmann transport formalism. This analysis highlights the role of inelastic electron-phonon interactions and higher-order quantum interference processes in generating asymmetric carrier scattering.

In parallel, we perform first-principles calculations of magnetic materials using Quantum ESPRESSO, Wannier90, and Perturbo. We calculate electronic band structures, Berry curvature distributions, and intrinsic anomalous Hall conductivity for ferromagnetic bcc iron and the kagome ferromagnet Fe_3Sn_2, a material known for its strong spin-orbit coupling and large anomalous Hall response. These calculations provide insight into the electronic origins of anomalous Hall transport and establish a computational foundation for future investigations of phonon-mediated extrinsic contributions.

Mathematically modelling neuronal circuit recovery through activity dependent myelination
Elizabeth J. Milne
Mentor: Michelle Effros

In "Unsupervised restoration of a complex learned behavior after large-scale neuronal perturbation", a paper by the Carlos Lois group, it was found that after genetic perturbation of the majority of excitatory neurons in the HVC, a brain region involved in song production, of zebra finches, the bird's song severely degraded, then fully recovered within two weeks. The mechanism behind this recovery is not completely understood; some network-level recovery mechanisms are proposed in the Lois group paper. In this report, we investigate the feasibility of potential recovery mechanisms operating within a very small neuronal circuit (involving 3 neurons), in particular the potential role of activity-dependent myelination. To do this, we utilize a mathematical framework developed by Effros and Li, which uses Markov chains to analyze the long-term behavior of neurons. By analyzing the long term behavior of the post-synaptic neuron with different statistical relationships between the two presynaptic inputs, we seek to find the conditions under which an unmanipulated neuron can adapt, via activity-dependent myelination, to compensate for a silenced neuron.

Design of a quantum bus for simultaneous all-to-all connectivity between superconducting qubits
Todor Miljevic
Mentors: Mohammad Mirhosseini, Frank Yang, and Parth Shah

Currently, superconducting quantum processors are inherently bottlenecked by quantum decoherence and connectivity limitations to nearest-neighbor only. Although quantum error correction combats decoherence, a far too large of a hardware overhead is required to actually implement it. The lab attempts to overcome both of the aforementioned bottlenecks by designing modular chips in such a way that simultaneous all-to-all connectivity is possible within each module. The lab demonstrates computationally an all-to-all modular qubit connection system using a resonator array scheme, which enables communication through evenly-spaced normal-mode frequencies centred around 5GHz. Along with demonstrating the array’s functionality using an electromagnetic solver, we predict its robustness to noise to be sufficient for tolerating up to 7MHz of frequency disorder per resonator.