



Physical Chemistry Experimental and Theory Graduate Student Award Symposium

3:00-5:50 p.m. EDT
September 17, 2021

Jeffrey DuBose, University of Notre Dame, Advisor: Prof. Prashant Kamat
Controlling Energy Transfer in Perovskite-Chromophore Complexes

Leopoldo Mejia Restrepo, University of Rochester, Advisor: Prof. Ignacio Franco
Mechanical Control of Charge Transport and Chemical Reactivity in Molecular Junctions

Dinumol Devasia, University of Illinois-Urbana-Champaign, Advisor: Prof. Prashant Jain
Label-free Tracking of Photocatalysis on Single Nanoparticles

Diptarka Hait, University of California-Berkeley, Advisor: Prof. Martin Head-Gordon
Orbital Optimized Density Functional Theory for Electronic Excited States

Abigail Dommer, University of California-San Diego, Advisor: Prof. Rommie Amaro
From Viruses to Sea Spray: Applications of All-Atom Molecular Dynamics to
Mesoscale Environmental and Biological Systems

Lauren McCarthy, Rice University, Advisor: Prof. Stephan Link
Investigating the Polarization-Dependent Scattering of Plasmonic
Nanoantennas Under Confined-Light Illumination

Hannah Katherine Wayment-Steele, Stanford University, Advisor: Prof. Rhiju Das
Theoretical Basis and Computational Design of Superfolder mRNA Therapeutics

Jeremy Schultz, University of Illinois-Chicago, Advisor: Prof. Nan Jiang
Probing Nanostructures on Surfaces at the Angstrom-Scale with Scanning
Tunneling Microscopy and Tip-Enhanced Raman Spectroscopy

Format: Two sessions will be held. In each session, four speakers will give 15-minute presentations, followed by a 20-minute panel Q&A.

Register in advance for Zoom Link:

https://us06web.zoom.us/webinar/register/WN_bgwNHQ4FRtKqWYKNSkGfHQ

Sponsors: Physical Chemistry Division of the American Chemical Society and The Journal of Physical Chemistry
Organizers: Experimental and Theoretical Physical Chemistry Subdivisions of the ACS. For questions contact
Prof. Jennifer Shumaker-Parry, shumaker-parry@chem.utah.edu

Jeffrey DuBose, University of Notre Dame

Controlling Energy Transfer in Perovskite-Chromophore Complexes

Summary: Controlling the flow of energy and the nature of the excited states that are produced in nanocrystal-chromophore hybrid systems is crucial for realizing their photocatalytic and optoelectronic applications. In this talk, we determine whether perovskite nanocrystals are sensitizing singlet or triplet excited states on rhodamine B molecules, then leverage the chemical tunability of the perovskite nanocrystals to determine the mechanism of energy transfer.

Dinumol Devasia, University of Illinois-Urbana-Champaign

Label-free Tracking of Photocatalysis on Single Nanoparticles

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Summary: In my research I utilized single-molecule-level vibrational spectroscopy to watch chemical events on a catalyst that is in action, in a realistic reaction medium. This led to the discovery of a rich profile of C-C bonded species formed from CO₂ reduction on silver nanoparticles under plasmonic excitation.

Lauren McCarthy, Rice University

Investigating the Polarization-Dependent Scattering of Plasmonic Nanoantennas Under Confined-Light Illumination

Summary: The polarization properties of fields such as evanescent waves and confined light in general strongly diverge from their freely-propagating counterparts, including potentially taking on cycloid-like trochoidal field motion. In this talk, I will describe how we utilized the scattering from single plasmonic nanoantenna systems to reveal an additional class of polarized light-matter interaction called trochoidal dichroism, which may be able to serve as a complement to techniques such as linear and circular dichroism.

Jeremy Schultz, University of Illinois-Chicago

Probing Nanostructures on Surfaces at the Angstrom-Scale with Scanning Tunneling Microscopy and Tip-Enhanced Raman Spectroscopy

Summary: This work focuses on the development and application of a hybrid technique that combines scanning tunneling microscopy (STM) and tip-enhanced Raman spectroscopy (TERS) to achieve subnanoscale investigations of molecular and material nanostructures at the fundamental level. By implementing these methods in ultrahigh vacuum and at cryogenic temperatures it becomes possible to study interactions and reactions with respect to atomic-scale environments.

Leopoldo Mejia Restrepo, University of Rochester

Mechanical Control of Charge Transport and Chemical Reactivity in Molecular Junctions

Summary: In this contribution, I discuss mechanical strategies to monitor and control conformational dynamics, reactivity, and transport coherence at the single-molecule limit. In the end, I present a novel microscopic theory of conductance histograms that allows the interpretation and prediction of conductance measurements in break-junction experiments.

Diptarka Hait, University of California-Berkeley

Orbital Optimized Density Functional Theory for Electronic Excited States

Summary: Orbital optimized density functional theory (OODFT) can be effective at modeling challenging excited states like charge-transfer states and core-level excitations, where time dependent DFT (TDDFT) qualitatively fails. I will discuss a recently developed method for reliably converging OODFT solutions without "variational collapse" down to the ground state, performance of OODFT for known benchmarks and its application in interpreting experimental transient X-ray/XUV spectra.

Abigail Dommer, University of California-San Diego

From Viruses to Sea Spray: Applications of All-Atom Molecular Dynamics to Mesoscale Environmental and Biological Systems

Summary: All-atom molecular dynamics simulations were used to model and simulate stable multi-million atom systems, including nanoscale marine aerosol particles and the SARS-CoV-2 viral envelope. Lessons from building big systems are applied to simulating a billion-atom SARS-CoV-2-laden respiratory aerosol to understand how aerosolized viruses retain viability during airborne transmission.

Hannah Katherine Wayment-Steele, Stanford University

Theoretical Basis and Computational Design of Superfolder mRNA Therapeutics

Summary: RNA chemical instability presents a fundamental limit on the shelf life of RNA-based therapeutics such as mRNA COVID vaccines, yet a given antigen has astronomically many synonymous messenger RNAs that will code for it, some of which we hypothesized could be more resistant to hydrolysis than conventionally-designed mRNAs. I will describe the development of a theoretical framework and computational methods for modelling RNA hydrolysis that we used to guide design of "superfolder" model antigens more resistant to hydrolysis, and whose predictions were experimentally validated, demonstrating that the shelf life of any RNA therapeutic may be extended 2-3 fold simply through sequence design.