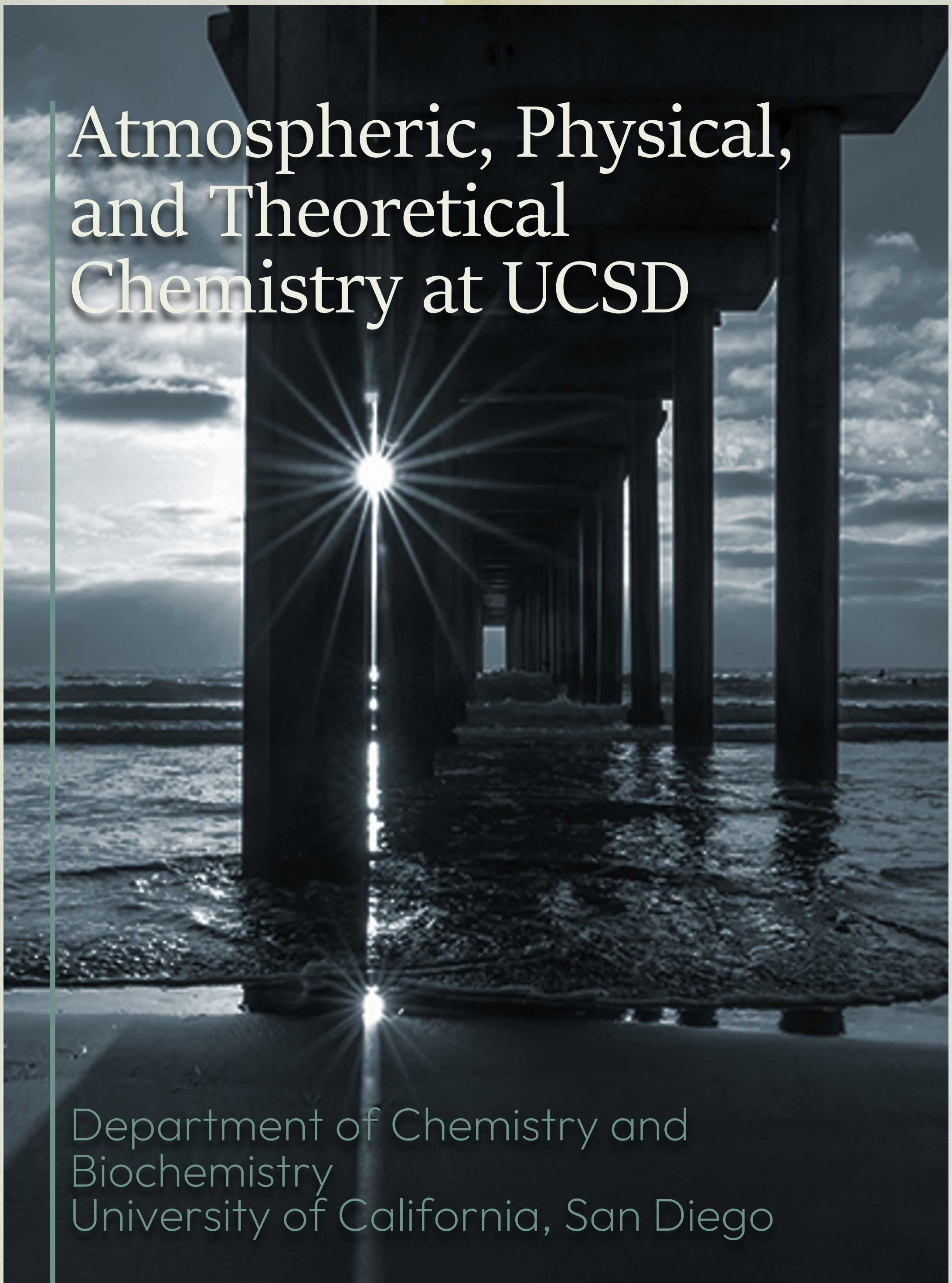
Atmospheric, Physical, and Theoretical Chemistry at UCSD



Department of Chemistry and Biochemistry
University of California, San Diego

Chemistry at UC San Diego

UC San Diego is a leading institution for scientific research. More than 50 faculty in the Department of Chemistry and Biochemistry perform research in a wide range of topics from atmospheric chemistry to molecular synthesis, structural biology, and materials research. It has been the home of many renowned scientists including Nobel laureates, Howard Hughes Medical Investigators, and members of the National Academy of Sciences.

Physical, Atmospheric and Theoretical Chemistry

The graduate program in Physical Chemistry at UC San Diego is ranked #17 in the United States by the US News and World Report 2023. The program draws on a strong interplay between theory and experiment in traditional and emerging areas of physical chemistry. Experimental techniques are developed and applied towards problems in energy storage and conversion, photonics and polaritonics, quantum and nanomaterials, biophysics, and reaction dynamics, with time resolution down to femtoseconds, and spatial resolution down to sub-nanometer. Current efforts in theoretical and computational chemistry are focused on topics such as quantum-mechanical methodologies for energy and electron transport, non-equilibrium statistical mechanics, biomolecular simulations, drug discovery, liquid phase dynamics in confined materials, and polariton chemistry. Atmospheric research in the lab and measurements in the field investigate key processes associated with aerosol chemistry, human health, and climate change.

Curricula

Physical Chemistry

Chem 231 *Chemical Kinetics and Molecular Reaction Dynamics* **Chem 239** *Special Topics in Physical Chemistry*	**Chem 230A** *Quantum Mechanics I* **Chem 232A** *Statistical Mechanics I*	Two courses among: **Chem 205B** *Analytical Chemistry II* **Chem 235** *Molecular Spectroscopy* **Chem 273** *Atmospheric Chemistry*

Analytical and Atmospheric Chemistry

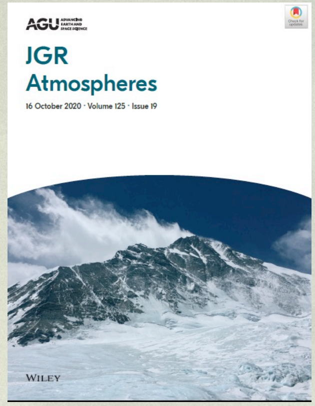
Chem 231 *Chemical Kinetics and Molecular Reaction Dynamics* **SIO 217A** *Atmospheric Thermodynamics*	Two courses among: **Chem 230A** *Quantum Mechanics I* **Chem 271** *Analytical Chemistry I* **Chem 232A** *Statistical Mechanics I*	Two courses among: **Chem 205B** *Analytical Chemistry II* **Chem 235** *Molecular Spectroscopy* **Chem 273** *Atmospheric Chemistry*

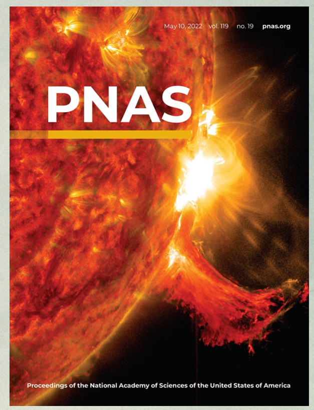
Theoretical and Computational Chemistry

Chem 239 *Special Topics in Physical Chemistry* **Chem 285** *Introduction to Computational Chemistry*	**Chem 230A** *Quantum Mechanics I* **Chem 232A** *Statistical Mechanics I*	Two courses among: **Chem 235** *Molecular Spectroscopy* **Chem 230B** *Quantum Mechanics II* **Chem 232B** *Statistical Mechanics II*

Atmospheric Chemistry

Thiemens Group (http://thiemensgroup.ucsd.edu/)





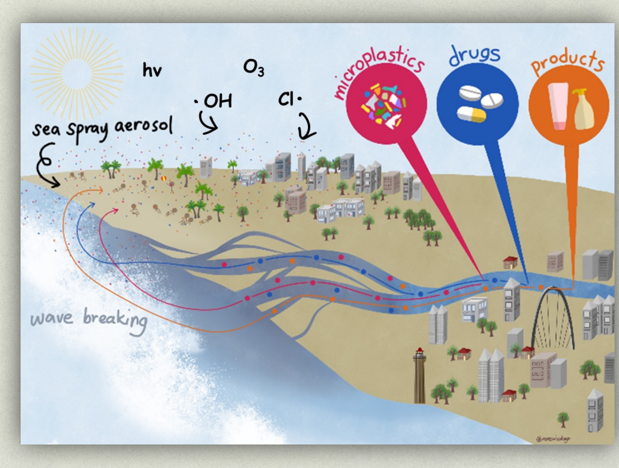
Our research uses stable and radiogenic isotopes to trace physical chemistry processes and natural phenomena over space and time. Using radioactive sulfur, we are determining melting rates of Himalayan ice, water resources to nearly half the world. We sample across Tibet and up to Mt Everest. For higher sampling we are developing a new rocket system to sample through the atmosphere to the edge of space. A new variety of near field nasoscope is being developed to analyze return extraterrestrial samples, such as comets and Mars. We study the quantum chemical processes using the Berkeley synchrotron and the fundamentals are applied to measurement of samples to study earths origin and evolution of life.

The Figure on left (JGR 2020), with former student Lin Mang is our field sampling on North face of Mt Everest. The picture of solar corona is our cover for paper (PNAS 2022) using radiogenic 35S to detect solar variations and El Nino events

Prather Group (https://kprather.scrippsprofiles.ucsd.edu/ & https://atofms.ucsd.edu/)

Research in the Prather group focuses on atmospheric aerosols and their impacts on air quality, climate, and human health. Our research involves lab and field studies, developing real-time instrumentation and sensors for environmental measurements, probing heterogeneous chemistry, mapping airborne pathogens, and studying ocean-atmosphere exchange of gasses and sea spray aerosols. We also focus on the environmental impacts of ocean-derived pollutants and toxins in pollution in coastal regions by developing a better understanding of the ocean-to-atmosphere transfer of pollutants and pathogens, subsequent atmospheric transport, and health impacts from airborne exposure and to inform and alert the public. We work collaboratively with a team of interdisciplinary scientists including the medical school and public health to better understand the impacts on human and ecosystem health under changing climate conditions. Ultimately, our goal is to develop solutions to societal challenges through bridging measurements with climate and air quality models to develop more effective policies.

Slade group (https://sites.google.com/ucsd.edu/slade-lab)

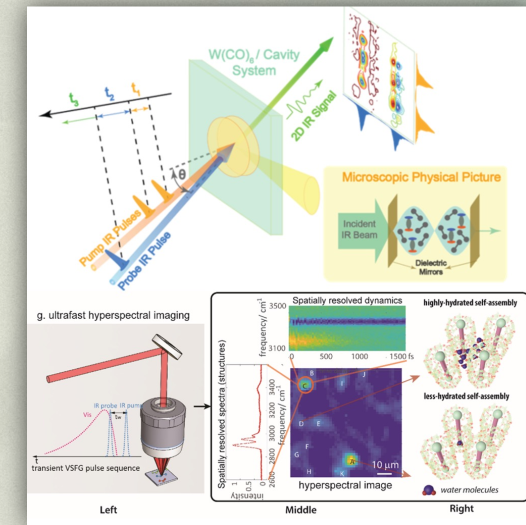


In the Slade group, we are broadly interested in how aerosols affect atmospheric chemistry, air quality, and climate. We study multiphase (gas and particle) processes that govern the fundamental properties (e.g., phase/viscosity and hygroscopicity) and chemistry of aerosol. Major efforts include (1) utilizing soft ionization mass spectrometry to examine reactions and the kinetics (rates) of reactions occurring on model sea spray aerosol surfaces, (2) quantifying chemical contaminants including plastic residues in real sea spray aerosol in the field, and (3) characterizing the emission characteristics and physicochemical properties of respiratory aerosols from speech. Our group collaborates with the UC San Diego NSF Center for Aerosol Impacts on Chemistry of the Environment (CAICE) and the School of Medicine. Our work has been supported by the NSF Atmospheric and Geospace Sciences (AGS) division, the US Environmental Protection Agency (EPA), and some of our graduate students have been supported by the NSF Graduate Research Fellowship Program (GRFP).

Physical Chemistry

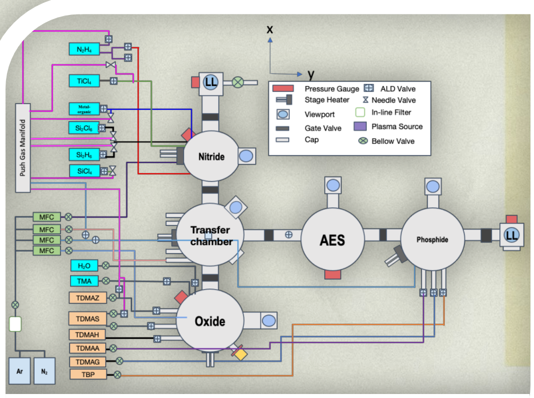
Xiong Group (http://ultrafast.ucsd.edu)

The Xiong group aims to controlling and understanding molecular structures and dynamics of materials, so that we can provide principles of designing materials with specific functions and properties. To achieve this goal, we develop ultrafast spectroscopic techniques that can track dynamics in frequency, time, and spatial domains, as well as implementing new light sources such as extreme ultraviolet (EUV) to gain element specificities. Specifically, we are interested in (1) applying and developing 2D IR spectroscopy to follow ultrafast dynamics of polariton chemistry, (2) developing vibrational sum frequency generation (VSFG) microscopy to resolve microscopic structures of soft material tissues, (3) developing table-top XUV spectroscopy to study ultrafast electron-hole dynamics in multiferroic materials, (4) using VSFG spectroscopy to follow electron transfer at energy material interfaces and study electrochemical reactions at catalytic surfaces, and (5) revealing water-host interactions in metal-organic-frameworks.



Kummel Group (http://kummelgroup.ucsd.edu)

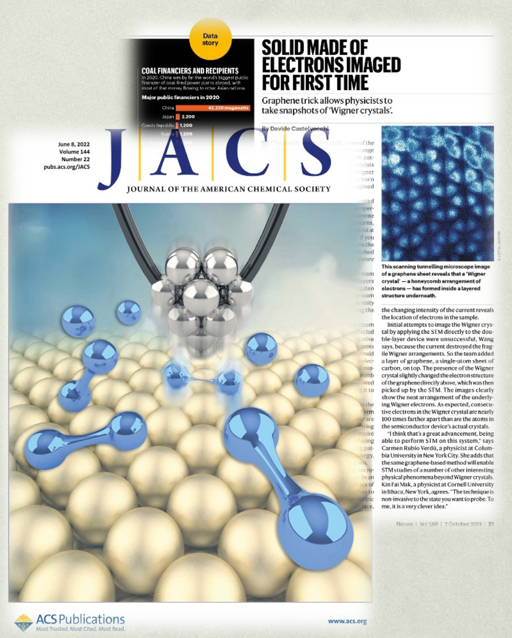
The Kummel group investigates the chemistry of microelectronic processing as well as coating of cancer drugs. For investigation of microelectronic chemistry, the primary tools are atomic layer deposition (ALD), chemical vapor deposition (CVD), bipolar sputtering, in-situ xray photoelectronic spectroscopy (XPS), transmission electron microscopy (TEM), ad ex-situ electrical measurements. The group seeks to correlate the control of the chemical and physical structure of thin films with their practical electrical properties. Projects include selective deposition of oxides, ALD for interconnects/contacts and packaging, ALD of gate oxides for CNTs and TMDs, CVD of low K dielectrics, and deposition of heat spreaders. The lab is funded by industry (Applied Materials, TSMC, EMD, Qualcomm, the Semiconductor Research Corporation, Rasirc, and Samsung) as well as DARPA so it is very focused on applied science. For the coating of cancer drugs, liposomal coatings of oncolytic viruses are being developed in collaboration with Epicentrx.



Cluster tool in the Kummel Lab. This is one of four tools which enable thin film deposition with in-situ analysis by Auger (AES) or Xray photoelectron spectroscopy (XPS)

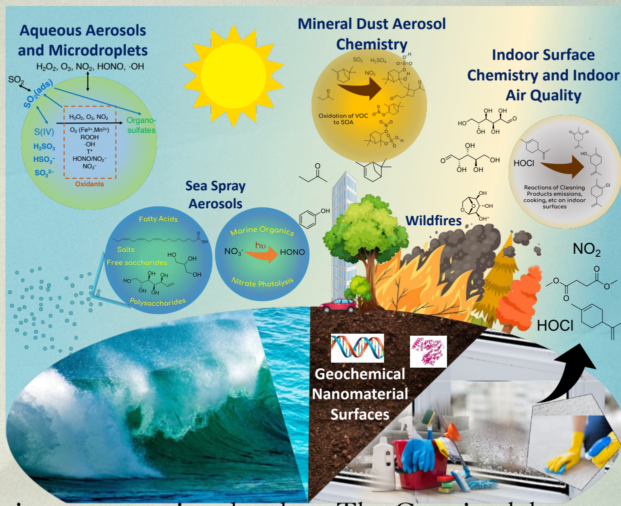
Li Group (https://sites.google.com/ucsd.edu/small)

The Spectroscopy and Microscopy at Atomic Level Laboratory (SMALL) led by Dr. Shaowei Li operates at nearly the fastest and the smallest scales people can achieve. It combines optical techniques with scanning probe microscopy (SPM) to explore the unconventional properties of low-dimensional quantum materials including single atoms, molecules, and 2D layered materials in both real and temporal spaces. The ultrafast optical spectroscopy allows the team to catch the transient motion of electrons and unclear that happens within a tiny fraction of a second. The SPM helps us capture a clear picture of materials with single-atom resolution. Coupling of photon excitation with electron tunneling at the junction of an SPM provides the team with a new window for viewing the unique properties of individual nano-scale objects compared to their bulk counterparts.

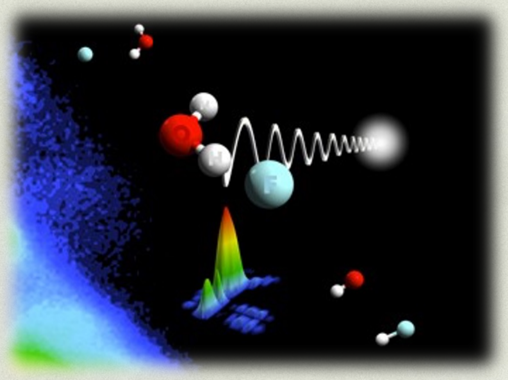


Physical Chemistry

Grassian Group



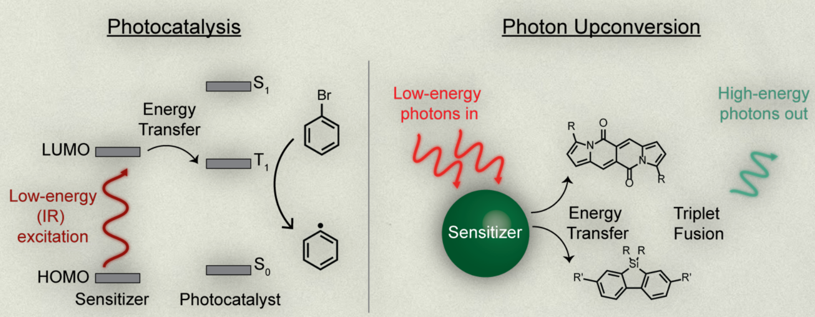
(https://sites.google.com/ucsd.edu/grassiangroup/home)
Research in the Grassian Group focuses on the chemistry of environmental interfaces and the use of molecular-based probes to better understand the global impacts of these interfaces. Environmental interfaces include atmospheric aerosols, engineered and geochemical nanomaterials, and indoor surfaces. Several ongoing projects include: understanding the molecular level details of the heterogeneous chemistry of trace gases with particulate matter such as mineral dust and sea spray in the atmosphere; sulfur oxidation and organosulfur reactions in aqueous aerosols; surface interactions and transformations of biological macromolecules, including environmental DNA (eDNA), on geochemical nanomaterial interfaces; the chemistry of indoor surfaces and their impact on indoor air quality and; chemistry at the air/water interface in aqueous microdroplets. The Grassian laboratory utilizes an array of state-of-the-art instrumentation including Aerosol Optical Tweezers, Atomic Force Microscopy coupled to Infrared Spectroscopy, Optical Photothermal Infrared Spectroscopy Incoherent Broadband Cavity Enhanced Absorption Spectrometer, Micro-Raman Spectroscopy, Quartz Crystal Microbalance-Dissipation, ATR-FTIR Spectroscopy and High-Resolution Mass Spectrometry, just to list a few.



Continetti Group (http://checont6.ucsd.edu)

Research in the Continetti group focuses on measuring and understanding the dynamics and energetics of transient species using photoelectron and photofragment imaging techniques. Production of highly excited neutrals by photo-detachment of negative ions and charge exchange neutralization of cations provide complementary approaches to studying the dissociation pathways and dynamics of a wide range of molecules and clusters. Using state-of-the-art mass spectrometry, ion trapping and coincidence techniques, processes ranging from dissociative photodetachment to three-body dissociation dynamics are studied in great detail. Current projects include: (a) Studies of the effects of vibrational excitation on transient combustion intermediates such as the HOCO radical; (b) Energetics and dynamics of oxygenated radicals important in biofuel combustion; (c) Effects of solvation on the energetics of model chromophores in photoactive proteins; (d) Development of an aerosol impact spectrometer for studying systems ranging from atmospheric aerosols and energetic materials to complex nanomaterials by hypervelocity impact on inert surfaces.

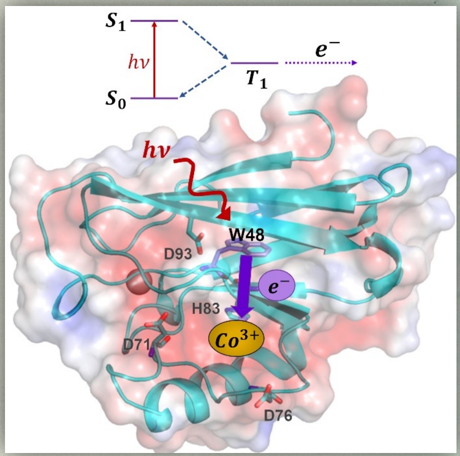
Pun Group



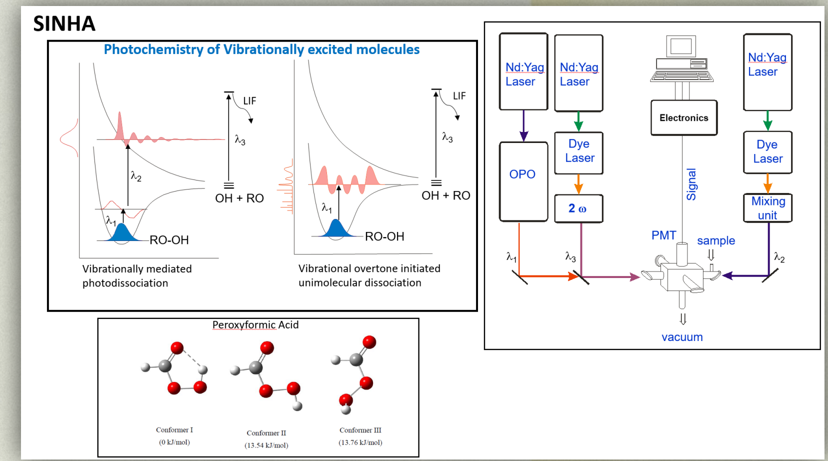
Research in the group of Andrew Pun focuses on studying the movement of excitons in semiconductor materials. We utilize organic, inorganic, and hybrid materials to carry out these goals. In particular, we are interested in studying compounds that can undergo photon upconversion or be used for photocatalysis. Upconversion is the process of converting low-energy photons into high-energy photons, and has broad applications from photovoltaics to 3D printing. Photocatalysis is the process of utilizing light to drive catalytic reactions, and has seen widespread attention in recent years with implications in medicinal chemistry as well as alternative energy. In addition, we are interested in studying exciton energy transfer, to optimize this key step in our other aims. Research in our group is highly interdisciplinary. Students will gain experience across a broad array of topics, ranging from synthetic chemistry to laser-based optical measurements.

Physical Chemistry

Kim Group (http://galileo.ucsd.edu/)



In our lab, photons and proteins meet to elucidate complex biochemical reactions. A project on membrane protein folding is inspired by fundamental questions about the mechanisms of insertion and folding, including the role of water and lipids during transfer to the bilayer. A second project on electron transfer elucidates the role of protein environment on the generation and stabilization of tryptophan radicals as intermediates for long-range charge separation. The figure shows the electron transfer reaction from tryptophan-48 in a blue-copper protein azurin and highlights the role of the triplet state in this photochemical reaction. Group members gain knowledge and valuable skills across a wide range of topics, including protein expression and purification, and many varieties of spectroscopic techniques such as absorption, emission, vibrational Raman, circular dichroism, and time-resolved (pump-probe).



Sinha Group

Research in the Sinha lab is directed towards using spectroscopic techniques and computational methods to investigate gas phase molecules with atmospheric relevance. On the experimental side, we use "action" spectroscopy to probe the vibrational overtone spectra and mode-selective behavior of hydroperoxide molecules. Hydroperoxides are an important class of atmospheric molecules as they are a major source of OH radicals. Our work on CH3OOH has shown that the rate of intramolecular vibrational energy redistribution (IVR), as well as the subsequent vibrationally mediated photochemistry of this molecule very much depends on which vibrational mode is excited. In more recent work, we have also used action spectroscopy to investigate the vibrational overtone initiated unimolecular dissociation of peroxyformic acid (PFA). Peroxyformic acid is interesting in that it exhibits internal hydrogen bonding. We have used laser induced fluorescence to probe the OH fragments resulting from the unimolecular dissociation of PFA excited to the 6νOH level and from this data have been able to provide stringent limits on the O-O bond dissociation energy and infer dissociation pathways. On the computational side our lab is interested in investigating the ability of atmospheric acids to catalyze various gas phase hydrogen atom transfer reactions.

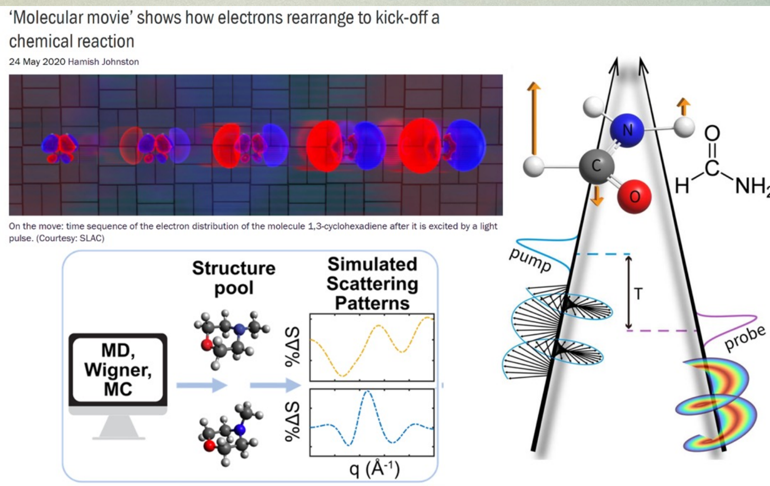
Tauber Group (http://tauber.chem.ucsd.edu/)

The Tauber group employs physical and analytical chemistry to gain insights into diverse systems that fascinate us and our collaborators. To mention some examples, we have explored dye-sensitized solar cells; excited-state dynamics of carotenoid aggregates and dimers; the coloration of bird feathers; photophysics of dissolved organic matter in ocean water; and mechanisms of electrical conduction in rocks at extreme temperatures and pressures. Researchers in our lab have used many different approaches to probe these systems, e.g., electrical measurements under simulated solar conditions; synthesis of organic molecular dimers; various spectroscopic methods including electron paramagnetic resonance (EPR), luminescence, absorption, Raman scattering, and impedance spectroscopy; and electronic structure calculations. Our lab also houses systems for performing advanced time-resolved measurements, specifically femtosecond transient absorption and picosecond resonance Raman spectroscopy.

Two neotropical birds probed using optical spectroscopy in the Tauber group. Arch. Biochem. Biophys. https://doi.org/10.1016/j.abb.2013.09.009

Physical Chemistry

Yong Group (https://sites.google.com/ucsd.edu/yong)

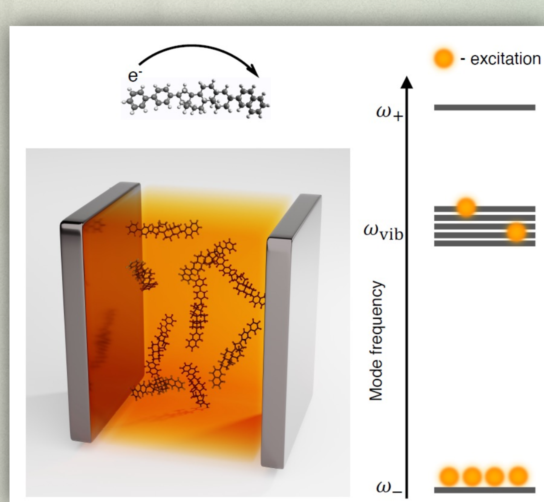


Research in the Yong Group focuses on developing novel experimental and theoretical techniques to study ultrafast light-induced processes in molecules. We aim to "watch" chemical reactions with atomic-scale spatial resolution and sub-femtosecond temporal resolution. This is expected to lead to new chemical reactions created through the control of atoms and electrons in molecules on ultrafast time scales. We conduct both experimental and theoretical studies in our group. Experimentally, we perform ultrafast x-ray/electron scattering experiments in gas and liquid phases using Synchrotrons, XFELs, and UED at national labs, with the goal of tracking ultrafast quantum motions of nuclei and electrons in molecules in both space and time. In our own ultrafast laser lab at UCSD, we conduct ultrafast molecular spectroscopy, including transient absorption spectroscopy, transient (magnetic) circular dichroism, time-resolved photoelectron imaging, and photoelectron circular dichroism, to study ultrafast processes such as dynamical chirality. Theoretically, we develop advanced tools for recovering desired molecular properties from measured data. Additionally, we design novel concepts for creating new photophysical/photochemical phenomena and new techniques that can reveal chemical information otherwise unavailable.

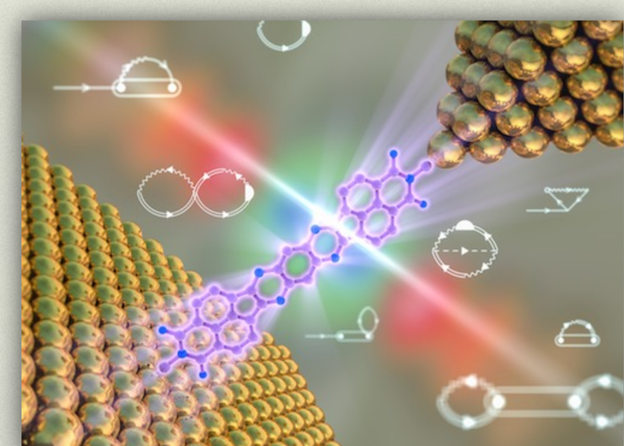
Theory & Computation

Yuen-Zhou Group (http://yuenzhougroup.ucsd.edu/)

Research in the Yuen-Zhou group explores theoretical and computational aspects of novel and unconventional light-matter interactions in the weak, strong, and ultrastrong coupling regimes. Current interests include the hybridization of light and ensembles of molecular vibrations or excitons in microcavities or more elaborate photonic architectures, and in the physicochemical properties and processes afforded by these hybrid architectures. Of much relevance in these studies are the exploration of emergent many-body physics of these systems such as Bose Einstein condensation, collective chemical reactivity, and novel phase transitions driven by light. Typically, students joining the Yuen-Zhou group have a proclivity towards mathematical derivations and proofs and will receive training in analytical and computational quantum and statistical mechanics, as well as in interdisciplinary topics concerning photonics and organic optoelectronics.



Vibrational polariton condensate



Galperin Group (http://galperingroup.ucsd.edu/)

Characterizing and controlling the response of open non-equilibrium molecular systems is crucial for the fundamental understanding of physical processes at the nanoscale as well as for developing more efficient nanodevices. Research in the Galperin group is focused on theoretical nanoscience, with emphasis on quantum charge, spin and energy transport, optical responses, and dynamics of open molecular systems. The Galperin group develops new techniques that connect molecular electronics with quantum chemistry, molecular spectroscopy, plasmonics, and quantum thermodynamics of nanoscale systems.

Theory & Computation

Sous Group

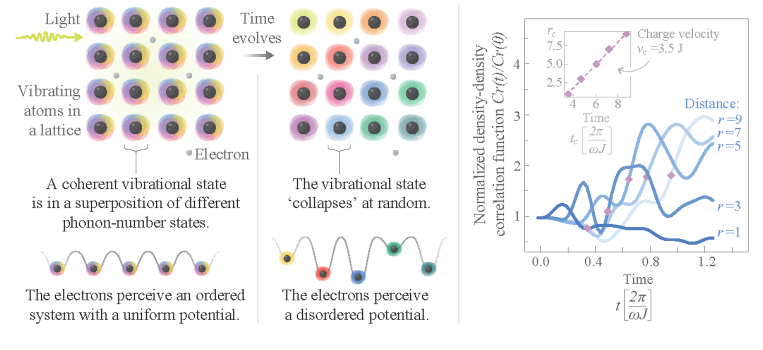
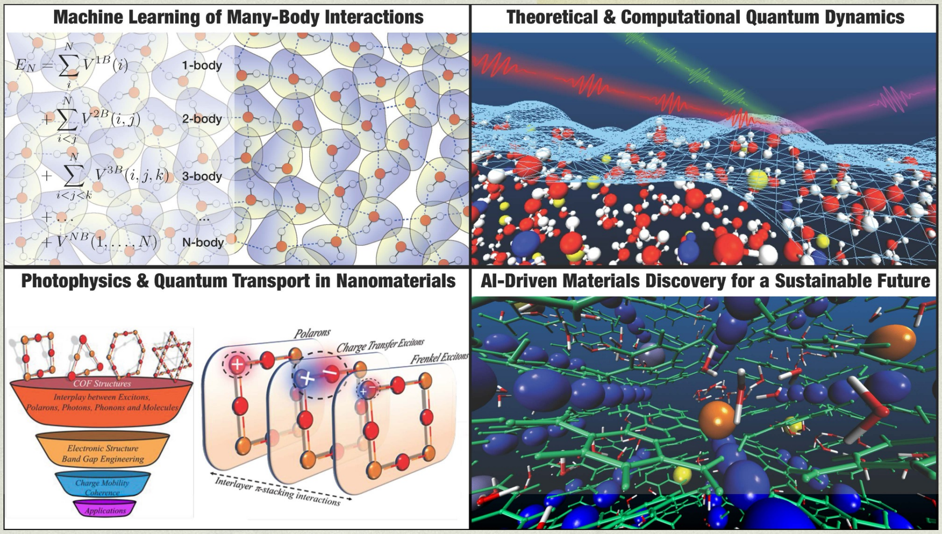


Figure 1: Dynamics of optically pumped metals. Left: Schematic of disorder generated by optically excited phonons in a metal. Right: Correlation function computed using tensor-product state approach.

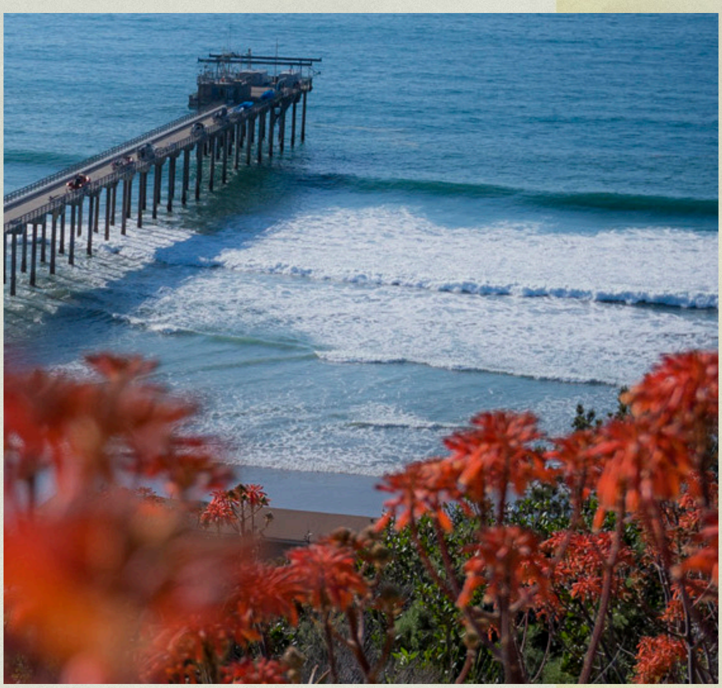
Research in the Sous group focuses on the study of systems in which quantum correlations between particles act to stabilize extreme states and sometimes entirely new forms of matter. We aim to gain a general, unifying understanding of interactions in many-body systems by studying model systems realized in experiments in some instances, or by identifying universal features common amongst many realizations in others. We study emergent states and phases in correlated quantum materials (e.g. superconductivity, correlated insulators, disordered metals, critical systems), ultracold atoms and molecules (such as Rydberg gases), dynamics of non-linearly and optically driven systems (e.g. in pump-probe experiments), and fundamental aspects of quantum information. My research relies on a carefully tailored combination of analytical and numerical techniques. To advance in this research, we develop theoretical concepts and numerical codes.



Paesani Group

(https://paesanigroup.ucsd.edu)

We are at the forefront of integrating artificial intelligence (AI) with quantum and statistical mechanics to unveil a new era of materials discovery vital for a sustainable future. Our research is divided into four intertwined domains: machine learning of many-body interactions for a realistic modeling of complex molecular systems, theoretical and computational quantum dynamics to unravel the behavior of molecules and materials at the quantum level, modeling of photophysical properties and quantum transport in nanomaterials to elucidate mechanisms that drive light-matter interactions in nanostructured materials, and AI-driven materials discovery to deploy advanced AI methodologies to accelerate the discovery and design of novel materials with unprecedented properties. Through the development, implementation, and deployment of new computational models, we aim to address global challenges in energy, environment, and health, bridging the gap between theoretical predictions and real-world applications. Our multi-disciplinary approach embodies a synergy of cutting-edge theories, computational techniques, deep physical insights, and a relentless pursuit of innovation, making significant strides towards a sustainable and technologically advanced future.



Life in San Diego

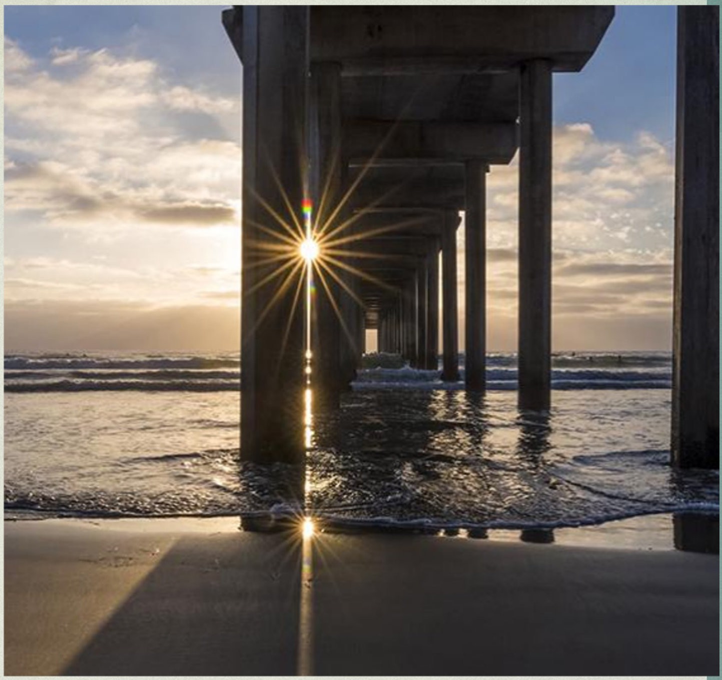
Considered one of the most beautiful cities in the world, downtown San Diego is just minutes from the UC San Diego campus. The campus is located in the seaside resort community of La Jolla (left image), one of the most spectacular beachfront communities in California. Recreational activities are abundant and the weather is beautiful year-round. UC San Diego Chemistry and Biochemistry invites you to experience the educational opportunities and a quality of life that rank among the best in the world!

How to Apply

Applicants for our Ph.D. and M.S. programs apply online. All applications to our program should include the following:

- UC San Diego application form
- Statement of purpose
- Three letters of recommendation
- Official transcripts
- Research experience or publications

You are also encouraged to contact the faculties about the details of their research. For complete information about the Department of Chemistry and Biochemistry, visit: http://chemistry.ucsd.edu.



We look forward to you joining us and becoming part of the UC San Diego team!