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. Our faculty include two Nobel laureates, three Howard Hughes Medical Investigators, and eight members of the National Academy of Sciences.

The graduate program in Physical and Atmospheric Chemistry at UC San Diego 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, materials, biophysics, medicine, and reaction dynamics. 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, proton conduction for fuel cell applications, ultrafast spectroscopy, and photochemistry. Atmospheric research in the lab and measurements in the field investigate key processes associated with aerosol chemistry and climate change. The Department is also home of the NSF Center for Chemical Innovation, Center for Aerosol Impacts on Climate and the Environment, which provides unparalleled research and teaching opportunities for graduate students.

http://chemistry.ucsd.edu
The research of the Prather group (http://atofms.ucsd.edu) focuses on increasing our understanding of atmospheric aerosols in air pollution, climate change, and health effects. To this end, members of the group conduct both field and laboratory studies as well as develop portable novel instrumentation. Current projects include: 1) Understanding how aerosols influence cloud formation and precipitation processes, 2) Characterization of atmospheric heterogeneous and multiphase chemistry, 3) Determination of mixing state, structure and climate properties of aerosols, 4) Understanding ocean impacts on clouds and climate. The Prather group couples aerosol and gas phase measurements with satellite data and climate models to derive a stronger understanding of aerosols chemistry. Members of the group use a unique instrument originally developed in the Prather lab (the aerosol time-of-flight mass spectrometer or ATOFMS), to perform measurements in remote locations, onboard research ships, and aircrafts.

The Thiemens group (http://thiemensgroup.ucsd.edu) focuses on understanding isotope effects at the quantum-mechanical level with application to both terrestrial and extra-terrestrial environments. This is made possible by measurements carried out at the South Pole, Greenland Summit, and Tibetan Himalayas, as well as by lab experiments performed on meteorite and lunar samples from billions of years ago. Projects underway include: 1) Study of aerosol formation and chemical transport using stable and radiogenic isotopes, 2) Investigation of past climates from ice cores, 3) Characterization of photochemical processes in the upper atmosphere, 4) Study of the origin and evolution of the solar system using extra-terrestrial samples from Mars and meteorites as well as lunar and solar wind samples. The photochemical studies are carried out using the Advanced light Source Synchrotron at Berkeley.

Our Department is home to the Center for Aerosol Impacts on Climate and the Environment (CAICE), an NSF Center for Chemical Innovation (http://caice.ucsd.edu). Within CAICE, Prather, Paesani, Thiemens, Pomeroy, and Tauber groups are working with researchers from the Scripps Institution of Oceanography and other institutions to explore the role of atmospheric aerosols in our changing climate from a fundamental chemistry perspective. Research focuses on the development of innovative experimental and theoretical tools for the study chemically complex systems. The Center provides unparalleled research and teaching opportunities for graduate students with a cross-disciplinary slant which includes fundamental chemistry, ocean biology, instrument development, science communication, and climate. Nobel Laureate Professor Mario Molina works closely with CAICE scientists to develop a more complete understanding of the fundamental processes involved in heterogeneous chemistry and ice formation. Prof. Molina has a major interest in developing innovative solutions to the climate change problem and establishing stronger links between science and policy.
The **Xiong group** ([http://ultrafast.ucsd.edu](http://ultrafast.ucsd.edu)) focuses on understanding the structure and dynamics of complex systems (nanoparticles, nanomaterials, and liquid interfaces) that are difficult to characterize due to their fast dynamics, nanoscale spatial dimensions, and coupling with the surrounding environment. To tackle these challenges, the Xiong group develops and applies novel ultrafast spectroscopic tools, which combine cutting edge concepts and techniques from chemistry and physics, including multidimensional spectroscopy, photoelectron spectroscopy, and high-harmonics generation. Current research involves the development of surface sensitive two-dimensional sum-frequency spectroscopy (2D-SFG) with specific focuses on: (a) Revealing the relationship between molecular conformation and charge separation dynamics in novel nanomaterials for energy applications; (b) Studying molecular structure and dynamics at complex air/liquid interfaces that are used as proxies of sea-spray aerosols as part of the core activities of CAICE (see section on “Atmospheric Chemistry”)

The **Tauber group** ([http://tauber.chem.ucsd.edu](http://tauber.chem.ucsd.edu)) is tackling the challenge of solar energy conversion. Most of our members concentrate on the physical chemistry and spectroscopy of organic chromophores. These dyes are at the heart of very inexpensive large-area photovoltaics that we, and many others, hope will be printed reel-to-reel in the years ahead. The Tauber group is particularly interested in the emergent properties that result from intermolecular interactions. Thus, organic chromophores that are self-assembled in aggregates or other assemblies, or in thin films, are typical samples that the Tauber group probes with electronic and vibrational (Raman) spectroscopy. One mechanism that has fascinated the Tauber group is singlet fission, whereby a singlet excited state partitions its energy to create two triplet excited states. This mechanism could significantly enhance the efficiency of some types of solar cells. Other research interests focus on the design and construction of large-area, high-efficiency dye sensitized solar cells. In all projects, diverse types of optical and magnetic spectroscopy are employed to gain a comprehensive understanding of mechanisms and devices.

The **Kummel group** ([http://kummelgroup.ucsd.edu](http://kummelgroup.ucsd.edu)) has projects which span semiconductor chemistry to cancer pathology in close collaboration with other faculty at UC San Diego and many other universities and industrial research labs. (a) Scanning tunneling microscopy and spectroscopy along with DFT modeling are employed to investigate chemical processes on the atomic scale for developing lower power computer chips via atomics layer deposition of high-k metal oxides on semiconductors. (b) Atomic scale studies are performed on monolayer films organic semiconductors for chemical sensing and functionalization of two-dimensional semiconductors such as graphene. (c) Nanoparticles are being developed and tested in vivo for contrast enhanced ultrasound to enable surgeons to accurately remove breast tumors thereby avoid second surgeries. (d) Novel software techniques are being developed to automate analysis of contrast enhanced ultrasound video of tumor tissue. Research in the Kummel group is highly multidisciplinary and involves students from four departments.

*Significant overlap exists with research programs in Theory and Computation as well as in Nanoengineering.*
Research in the **Continetti group** (http://checont6.ucsd.edu) 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 HO2CO 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.

Research in the **Sinha group** (http://sinhagroup.ucsd.edu) is directed towards investigating state-resolved reaction dynamics of gas-phase molecules. The selectivity achieved in both the reactant state preparation and product detection steps allows to nullify the influence of thermal averaging and obtain detailed state-to-state data that are crucial for testing prevailing theories about the dynamics. A particularly exciting research area of current interest involves examining the influence of molecular vibrations on various chemical processes such as photodissociation, unimolecular reactions, and bimolecular reactions. In addition to dynamics, basic questions regarding the spectroscopy of vibrationally excited molecules are also of interest and analysis of “action” spectra, generated by monitoring the yield of a specific reaction product while scanning the frequency of the vibrational excitation laser, is used to glean information about the intramolecular interactions that control the flow of energy within the energized molecule.

The focus of the **Kim group** (http://galileo.ucsd.edu) research is biophysical investigations of two complex processes in biology: membrane protein folding and long-range electron transfer reactions. The overarching goals are to elucidate general mechanisms of in vitro protein insertion and folding into bilayers, and to identify key proton and electron transfer pathways that enable long-range, multi-step charge separation in proteins. Time-resolved and steady-state electronic, vibrational, and magnetic techniques are utilized to probe the photophysics, structures, and photochemistry of model protein and peptide systems. The ultimate goal is to combine the lessons learned from membrane protein folding and long range charge separation to elucidate one of the most important and challenging problems in biology: electron transfer across membranes.
The Yuen-Zhou group is a new research team (starting on July 2015) focused on the theoretical description of novel quantum and semiclassical phenomena at the interface of chemical, condensed matter, and materials physics. Research in the Yuen-Zhou group involves close interactions with experimental groups. Current projects include: (a) The photophysics and photochemistry of molecular aggregates and polymers under coherent and incoherent illumination; (b) Novel ways of transporting energy in hybrid organic-inorganic systems (excitons, plasmons, polaritons) via “topological” ideas; (c) Heuristic and formal methods to attack unsolved quantum chemistry problems using density functional theories and effective Hamiltonians; (d) Foundations of quantum mechanics and thermodynamics including Berry’s phases, thermalization, and entanglement in many-body closed and open systems.

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 (http://galperingroup.ucsd.edu) 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 small-scale systems.

The Paesani group (http://paesanigroup.ucsd.edu) develops new “first principles” methods for molecular-level simulations of condensed-phase systems. Combining machine-learning techniques with accurate quantum dynamics approaches, the Paesani group is interested in modeling heterogeneous chemistry on aerosol surfaces within the core activities of CAICE as well as complex chemical processes in porous materials. Current projects include: (a) Many-body approaches to molecular simulations; (b) Computational modeling of nonlinear vibrational spectroscopies through equilibrium and nonequilibrium quantum-dynamics methods; (c) Proton conduction in novel materials for fuel cell applications; (d) Electronic and magnetic properties of porous materials. Members of the Paesani group are actively involved in the development of next-generation software for molecular simulations through collaborations with NVIDIA and the developers teams of OpenMM and Amber.

Research projects in the Weare group include the development of thermodynamic models of geochemical processes and simulations of enzymatic reactions and solid/liquid interfaces. Graduate students participate in the development of high performance simulation methods, working with some of the major producers of modern simulation technology designed for implementation on massively parallel supercomputers. By understanding the theory and numerical algorithms that make the methods work, students are in a unique position to develop their own models to treat complex problems encountered in new technologies.
The **Amaro group** ([http://amarolab.ucsd.edu](http://amarolab.ucsd.edu)) is broadly concerned with the development and application of state-of-the-art computational and theoretical techniques to investigate the structure, function, and dynamics of complex biological systems. At the interface of chemistry, biology, physics, and pharmacology, our research integrates both applied and basic science components, with goals to bridge the interface between basic and clinical research. Emerging efforts in multi-scale modeling, especially at the interface of Brownian and molecular dynamics, and the integration of data from electron microscopy and tomography experiments into atomic level modeling, are tightly coupled to a wide range of biochemical and biophysical experiments that allow us to engage in dynamic and exciting collaborations with various experimental labs. The Amaro group is actively pursuing disease-related and biophysical research for human African trypanosomiasis, influenza, chlamydia, and cancer, and routinely interface with biologists, biochemists, and chemists across campus, as well as through national and international collaborations.

The **McCammon group** ([http://mccammon.ucsd.edu](http://mccammon.ucsd.edu)) has projects that range from theoretical physical chemistry to computational modeling of biomolecular and cellular activity. The focus of one cluster of projects is the application of computer simulations to understand the nature of calcium ion pumping by proteins in heart muscle cells, and how the resulting fluctuations of calcium ions drive heart muscle contraction. In addition to deepening our understanding of how the heart works, the results provide a valuable platform for physics-based discovery of new medicines for heart disease. More fundamental work on aqueous solvation and molecular recognition naturally evolves from these biophysical studies. Work in the McCammon group is highly collaborative, with ongoing collaborations with UCSD faculty in mathematics, chemistry and biochemistry, and pharmacology. The McCammon group has trained more than 60 graduate students, some of whom have gone on to faculty positions at universities such as Harvard, University of Michigan, University of Toronto, and Washington University. Others have become established at National Laboratories or at companies such as Amgen, Dow Chemicals, and Johnson & Johnson.

The **Lindenberg group** ([http://hypathia.ucsd.edu](http://hypathia.ucsd.edu)) is interested in understanding the origin, nature and consequences of the interactions of physicochemical systems with their environment. The Lindenberg group is particularly interested in the thermodynamics of small systems in which fluctuations may play an important role, with a specific focus on reaction-diffusion systems. Approaches used by the Lindenberg group to solve these problems combine analytic and numerical methods, with emphasis on the simplest possible generic models that illustrate a behavior of interest. The Lindenberg group is currently involved in a large project including an interdisciplinary team of scientists at UC San Diego composed of physicists, biologists, chemists, bioengineers and psychologists to investigate the dynamic principles of collective brain activity.

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**Significant overlap exists between the Theory and Computation program and research programs in Atmospheric Chemistry, Energy & Materials, Quantitative Biology, Physics, Applied Mathematics, and Computer Science. Students in the Theory and Computation program are also eligible for a formal degree in Computational Science through the CSME program.**
## Analytical and Atmospheric Chemistry

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## Theoretical and Computational Chemistry

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## Notes
- Chem 500 Teaching
- Research
Fun in San Diego
San Diego and the surrounding areas are abound with recreational opportunities. Whether you enjoy surfing, the opera, skiing, or the alternative music scene, San Diego has it all. You can go for an air balloon ride or skydiving just minutes from our campus! At UC San Diego you will never be bored inside or outside the lab.

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
• GRE scores on verbal, quantitative, analytical, and subject tests
• Research experience or publications

For complete information about the Department of Chemistry and Biochemistry, visit: http://chemistry.ucsd.edu.

A View of San Diego, California
Considered one of the most beautiful cities in the world, downtown San Diego (pictured above) is located just minutes from the UC San Diego campus. The campus is actually located in the seaside resort community of La Jolla (image below), one of the most spectacular beachfront communities in California. Recreational activities are abound 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!

To apply:
http://chemistry.ucsd.edu/graduate-program/admissions

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