Sample UCI Chem-SURF Research Projects

Selected profiles of Faculty Mentors are included below in alphabetical order. All of these Faculty Mentors have been successful in mentoring undergraduate researchers, including Chem-SURF students, in recent past. The references cited at the end have been specifically chosen to highlight accomplishments by undergraduate student researchers, including previous Chem-SURF participants. The applicants should note that this is not a full list of potential Faculty Mentors. The full list of all Chemistry Faculty are eligible to be Chem-SURF faculty mentors that can be found on the Chemistry Department website.

Clicking on the name of the Faculty member will take to their research website

Ioan Andricioaei, Professor, Chemistry: ***1) Enhanced Sampling in Trajectory Space.*** Many important equilibrium and kinetic properties of chemical systems (including proteins and nucleic acids) can be cast in terms of paths in multi-dimensional spaces. We see fertile ground for theoretical and computational work on several categories of paths, from chemical-reaction paths to paths in the sequence space of evolving proteins. We have developed a set of trajectory reweighting techniques based on a stochastic path integral formalism that is particularly useful to treat both computer simulations and single-molecule experimental traces. ***2) Computer Simulations of DNA-Binding Machines.*** Protein-DNA interactions are essential in such crucial cellular functions as replication, repair, transcription or recombination. Many enzymes at and ahead of the replication fork affect large DNA fragments. For instance, topoisomerases undo DNA knotting. Others, like helicases and polymerases, are biomolecular motors: they use the energy of binding and/or hydrolysis of nucleotides to do mechanical work on the DNA fragments to which they bind. Another example is the machinery that compacts DNA inside the capsid of viruses. We have an avid interest in the theoretical description of these fundamental genetic processes through massively parallel computer simulations. ***3) Dynamics-Function Relationships.*** An accurate measure of free energy, important for protein/RNA stability or ligand binding, has to include the entropy manifested in molecular flexibility. On the experimental side, this dynamic aspect is brought in by developments in solution NMR spectroscopy, which measures motion by relaxation experiments. Molecular dynamics simulation is an important tool to complement these measurements and to connect dynamics to entropy. Undergraduate research involves running molecular dynamics simulations of DNA, RNA, and/or proteins, visualizing (e.g., making movies of the molecules in motion) and analyzing the simulation data.

Maxx Arguilla, Assistant Professor, Chemistry: ***Chemical and Dimensional Control Over Optoelectronic States in Low-Dimensional van der Waals Solids***. The *Maxx X Lab* (MXLab: Experimental Low-Dimensional Condensed Matter Chemistry Laboratory) is an interdisciplinary chemistry laboratory at the interfaces of solid-state chemistry, materials chemistry and physics, and nanoscience. Research in the *MXLab* focuses on the chemistry and physics of novel solids from the bulk and down to the nanoscale. With such materials platforms, the understanding of emergent electronic, optical, magnetic, and quantum phenomena is realized by creating new solid-state materials that are comprised of weakly-bound subunits (*via* van der Waals forces) possessing reduced dimensionalities—in one- or two-dimension/s—and high surface areas. Since its establishment in September 2020, three undergraduate researchers have already joined the MXLab—all working (in-person and remotely) towards the common goal of creating the next generation low-dimensional solids and understanding their physical properties approaching the sub-nanometer size regime. In-person projects for undergraduate students in the MXLab include: **(1)** exploratory solid-state synthesis to probe the atomic-scale dimensional transition in metal chalcogenides, **(2)** understanding the surface chemistry and confinement effects in optically-active van der Waals lattices *via* solution-phase exfoliation, and **(3)** chemical vapor deposition of electronic and magnetic van der Waals nanowires and monolayers. Students will be trained on the necessary laboratory and synthetic techniques and no prior research experience is required.

Shane Ardo, Associate Professor, Chemistry, Chemical & Biomolecular Engineering, Materials Science & Engineering [*Cardon et al.*, 2020; *Tkacz et al.*, 2017]: ***Innovators in Clean Water and Renewable Energy Research***. The Ardo Group is a Team of Innovators that invent new ways to leverage daily variations in sunlight to help close the Water Cycle, Carbon Cycle, and Hydrogen Cycle. More specifically, the central aim of the Ardo Group research program is to understand and control dynamics of non-equilibrium processes relevant to desalination, atmospheric water harvesting, oceanic carbon capture, solar fuels devices, photovoltaics, electrolyzers, and fuel cells. Several undergraduate student research positions are available in the group related to understanding structure-property relationships in (i) ion-conducting polymers via continuum-level numerical modeling of their transport and reactivity properties; and (ii) doped metal-oxide perovskite photocatalyst nanoparticles for solar water splitting in cost-effective particle suspension reactors. In the nearly eight years since the inception of the Ardo Labs, more than 20 undergraduate and high school students have worked on these and related projects. Collectively, this work includes opportunities in materials synthesis, synthesis of organic molecules, electrochemical and photoelectrochemical characterization, device fabrication and evaluation, and numerical modeling.

Kieron Burke, Chancellor's Professor, Chemistry & Physics [*Li et al.*, 2016; *K Vu et al.*, 2015]: ***Development of Density Functional Theory: From warm dense matter to difficult chemistry, using mathematical physics and machine learning.*** We have federally funded projects to find density functionals using machine learning methods, to develop DFT for matter under extreme conditions, and to improve functionals for strong correlation We currently use kernel ridge regression to develop highly non-local functional approximations that can be made arbitrarily accurate with sufficient training. Recent undergraduates (Isabelle Pelaschier, Kevin Vu) have published papers [*Li et al.*, 2016; *K Vu et al.*, 2015]. Undergraduates should have taken a basic course in quantum mechanics (either physical chemistry or modern physics) and should have a working knowledge of Mathematica or Python. Professor Burke has a long history of involving many undergraduates from different fields in his research and most continue to excellent graduate programs in their subjects.

Annmarie Carlton, Professor, Chemistry [*Carlton et al.*, 2020; *Carlton et al.*, 2014]: ***Atmospheric Multiphase Chemistry***. Most particles in the atmosphere are not directly emitted; rather precursor gases undergo chemical transformation during transport. Untangling the physicochemical complexities to understand sources, chemical pathways, fate and transport requires knowledge and application of field, laboratory and modeling experiments. Undergraduate students are sometimes paired with a graduate student and repeat their experiments for quality assurance. Some undergraduates lead their own research, typically in groups, and this has led to publications in peer-reviewed literature and presentations at national and international meetings. Dr. Carlton has involved 10 undergraduates from different majors (chemistry, meteorology, environmental science, physics, engineering, computer science and business) in her research and contributed to publications and in public outreach to create air quality aware communities. Carlton group alum undergraduate researchers now excel in professional and academic graduate positions.

John Chaput, Professor, Chemistry and Pharmaceutical Sciences. Please refer to the website (https://chaputlab.com/) for the details of the ongoing projects.

Robert Corn, Professor, Chemistry: ***On-Chip Biosynthesis and Self Assembly of Protein Microarrays for Biosensing and Biotechnology***. The multiplexed detection of protein and microRNA biomarkers with microarrays has exploded onto the biosensor scene over the past decade. Label-free multiplexed detection methods such as surface plasmon resonance imaging (SPRI) have achieved sufficient sensitivity (picomolar or femtomolar concentrations); however, all of these methods typically require the fabrication of high fidelity microarrays of purified proteins or antibodies. Our research group has been developing on-chip fabrication strategies for the creation of protein microarrays that utilize a combination of templated biosynthesis (cell-free in vitro translation and transcription, IVTT) and subsequent self-assembly of the protein microarray on the SPRI chip for immediate use in SPRI surface bioaffinity measurements. As part of the proposed REU project, the Chem-SURF Fellow will create and verify novel surface attachment strategies for protein microarrays using Zinc finger fusion protein tags. In addition to learning the IVTT and other biochemical methods, the fellow will acquire knowledge in FTIR, XPS and SPRI surface analysis.

Vy Dong, Professor, Chemistry [*F. A. Cruz et al.*, 2016; *Faben A. Cruz et al.*, 2017; *Kim et al.*, 2017]: ***Development of Transition Metal-Catalyzed Transformations.*** Students in the Dong Lab focus on mastering physical organic chemistry concepts, including reaction mechanism, kinetics, and thermodynamics, with the ultimate goal of becoming experts in molecular design and construction. The REU student will be paired with a graduate or postdoctoral fellow mentor to work on designing a new catalyst, reagent, or total synthesis. Remote work will focus on a thorough literature search on the topic of interest, writing a review article for publication, and presenting the concept for feedback by the end of the summer. Computational work may also be pursued to aid the proposal idea. Depending on the situation, in person work will provide an opportunity to gain fundamental skills in preparing, isolating, and characterizing organic molecules. The REU student will become familiar with analytic instruments, including IR, NMR, and mass spectrometry. There may also be an opportunity to work on collaborative projects involving the design of building blocks and functional molecules for the evolution of enzymes and 3D multiomics. Ultimately, we aim to apply innovative catalysts, reagents, and synthetic strategies to contribute to the discovery of new medicines, fuels, and materials.

William Evans, Professor, Chemistry: ***Synthetic f Element Chemistry: Learning to Handle Air-Sensitive Materials***. Tradition has held that the f orbital metals (lanthanides and actinides) had a limited chemistry because their f valence orbitals lacked the necessary radial extension of d orbital metals. Although the chemistry of these metals is now recognized as extensive, experimental difficulty in handling these air-sensitive compounds has limited their investigation. This project will introduce undergraduates to f orbital chemistry and to the special lab methods needed to handle complexes highly reactive with oxygen and water. The f elements will also be with us for thousands of years in the form of radioactive waste products; so, it is important to interest students in this area and train them in the necessary techniques, using nonradioactive model systems. Given the difficulty of working with these elements, this project is narrowly focused to foster publishable results in the time available. In this project, the students will synthesize a series of (C5R5)3M complexes (R = H, alkyl, phenyl, silyl) as potential precursors to [(C5R5)3M]1- compounds containing new Ln2+ ions recently discovered in our lab. We will evaluate the stability of the Ln2+ complexes as a function of the R5 substituent set. The most stable complexes will be studied further in terms of their physical properties and particularly their magnetism. The Evans laboratory has trained a large number of outstanding undergraduate researchers, who have continued their studies at the Ph.D. level.

Celia Faiola, Assistant Professor, Chemistry and Biological Sciences [*Faiola et al.*, 2018; *Faiola et al.*, 2019; *Mehra et al.*, 2020]. ***Chemometric analysis of biogenic volatile organic compound emissions from tropical plants and alpine shrubs***. Plants release a complex mixture of volatile organic compounds (VOC) to the atmosphere. These compounds are highly reactive and participate in important atmospheric chemistry processes, such as formation and growth of atmospheric particles. The detailed chemistry of a few representative plant VOC compounds has been studied in the laboratory, but those may not necessarily serve as good model compounds for emissions from all plant types. This project will focus on surveying plant VOC emissions from two important plant types that have not been the focus of previous studies: tropical plants frequently used in landscaping in Southern California and alpine shrubs that have rapidly expanding ranges due to climate change. Chemometric analysis of the complex plant VOC mixtures will be performed to compare the VOC emission profiles between plant types. The REU student will learn to set up dynamic branch enclosures to sample VOC emissions, run samples on a thermodesorption gas chromatograph quadrupole mass spectrometer, and analyze the data using both univariate and multivariate statistical techniques. Dr. Faiola has mentored 11 undergraduate researchers in her laboratory, and has assisted 6 undergraduate researchers with writing proposals to acquire their own funding. She is working with 2 undergraduate researchers currently on first-author publications based on their research.

Sarah Finkeldei, Assistant Professor, Chemistry [*S Finkeldei et al.*, 2017; *S Finkeldei et al.*, 2020; *S C Finkeldei et al.*, 2019]. Our research takes place at the interface between chemistry and materials science to contribute solving challenges of the nuclear fuel cycle. We are studying complex oxides, such as $Nd_2Zr_2O_7$ pyrochlores, which are considered as potential nuclear waste form for the safe disposal of radionuclides in a deep geological repository. We have openings for students in the lab to help with the synthesis and characterization of these potential nuclear waste forms to study how they would respond to e.g. irradiation due to the immobilization of radionuclides. We are also interested in the thermal properties of complex oxides, i.e. nuclear waste forms, but in particular in the thermal properties of advanced nuclear fuels to enhance the safety and efficiency of modern nuclear fuels for energy generation by nuclear power plants. We have a second opening for a student that is interested in supporting a graduate student in the thermal conductivity analysis of these materials. Some familiarity with Python and numerical modeling would be advantageous.

Barbara Finlayson-Pitts, Distinguished Professor, Chemistry [*Ezell et al.*, 2019; *Vander Wall et al.*, 2020; *Wingen and Finlayson-Pitts*, 2019]. Please refer to the website (https://sites.uci.edu/finlaysonpittslab/) for the details of the ongoing projects.

Fillmore Freeman, Professor, Chemistry [*Freeman et al.*, 2013; *Freeman et al.*, 2012]: ***Computational Quantum Chemistry Investigations of Structures, Reaction Mechanisms, and Molecular Rearrangements***. High levels of modern electronic theory are used to increase our understanding of structures, reaction mechanisms, molecular rearrangements, and solvation in the areas of bioorganic, inorganic, medicinal, organic, and organometallic chemistry. The REU student will be introduced to the fundamental concepts and principles of computational organic quantum chemical calculations in order to elucidate the mechanisms of 1,3-dipolar cycloadditions, 1,2- and 1,4-additions to 1,3-dicarbonyl compounds, cyclocondensations, and the chemistry of amino acids, peptides, sulfenic acids, and selenenic acids. Professor Freeman has mentored more than 200 undergraduate researchers. Many of them are coauthors, made presentations at local, regional, and national scientific meetings, won prestigious research awards, and attended graduate schools and professional schools.

Filipp Furche, Professor, Chemistry [*Furche et al.*, 2016; *Johansson et al.*, 2014; *Langeslay et al.*, 2017; *Palumbo et al.*, 2018; *R. C. Steinhardt et al.*, 2017; *Tao et al.*, 2018; *Vincent et al.*, 2016]: ***Theoretical and Computational Method Development and Chemical Applications***. While electronic structure calculations have become widespread in chemistry, very few students have the opportunity to look behind the scenes and understand the inner workings of electronic structure codes. Undergraduate students in the Furche group have the opportunity to explore the connection between quantum theory, high-performance computing, and chemistry in a supportive and collaborative environment. From the very beginning of their REU project, students will be immersed into research projects currently pursued by the Furche group in a team together with other undergraduates, graduate students, and postdocs. Current research directions include the development of new methods to solve the electronic Schrödinger Equation from first principles efficient and general enough for wide application to chemistry, non-adiabatic molecular dynamics methods, as well as applications in collaboration with experimental chemistry groups at UCI. Students will work in a UNIX environment and be introduced to scientific programming, use of high-performance computers, and scientific software. In the past few years, several undergraduates have co-authored publications, and three have been accepted to renowned graduate programs in theoretical and computational chemistry.

Alon Gorodetsky, Assistant Professor, Chemistry; Chemical Engineering and Materials Science: ***Cephalopod Proteins***. Cephalopods are known as the chameleons of the sea – they can alter their skin's coloration, patterning, and texture to blend into the surrounding environment. These capabilities are enabled by unique proteins and self-assembled nanostructures found within cephalopod skin. Our group is exploring new types of photonic and protonic devices from naturally occurring materials found in cephalopods. Our findings hold implications for the next generation of camouflage and renewable energy technologies. The Gorodetsky Group has an extensive track record of mentoring undergraduate student researchers. A total of 12 students from various majors have worked in the lab between 2011 and 2013 The Gorodetsky Group has specifically focused on the recruitment of individuals from disadvantaged and STEM underrepresented groups; the twelve students include 3 females and 4 Hispanic students, as well as 3 economically disadvantaged transfer students from community colleges. These undergraduate researchers have been supervised by senior graduate students and postdocs, but have also been granted quite a bit of independence. Indeed, the students develop and evaluate their own experimental strategies, participate in group meetings, present at local conferences, contribute to published work, and prepare proposals for fellowships. The success of our internal undergraduate research and training program is supported by several pieces of evidence: 1) 10 of the 12 students have received either Undergraduate Research Opportunity Program (UROP) or Research Experience for Undergraduates-like fellowships based on independently written and conceptualized proposals. 2) 2 of the 12 students are listed as co-authors on journal articles, and 4 other students are co-authors on manuscripts in the early stages of preparation; 3) 5 of the 12 students have already applied to graduate school, with two receiving acceptance notices.

Zhibin Guan, Professor, Chemistry: ***Biomimetic Modular Polymers for Advanced Biomaterials***. To mimic the modular domain structure of structural biopolymers such as the muscle protein, titin, our lab is developing polymers with a linear array of modules held together by programmed intramolecular weak interactions. Single-molecule nanomechanical studies demonstrate our biomimetic concept's feasibility: introducing modular structures held by sacrificial weak bonds into a polymer chain can combine in one polymer the three fundamental mechanical properties: high tensile strength, toughness and elasticity. We will investigate these polymers at single-molecule and macroscopic scales for their strength, toughness, and elasticity. An REU Fellow will participate in the synthesis of intermediates for the modules and gain experience in organic and polymer synthesis, molecular characterization, single molecule studies using Atomic Force Microscopy (AFM), and bulk physical property studies by MTS and DMAT. The Guan laboratory includes a number of undergraduates, and former students from his laboratory have pursued successful graduate and scientific careers; he currently has three undergraduates working in his group.

Alan Heyduk, Professor, Chemistry: ***Electronic Structure of Redox-Active-Ligand Transition-Metal Complexes***. The Heyduk group is developing new transition metal complexes of redox-active phenylenediamine and aminophenol ligands to apply their electron reservoir capabilities in new stoichiometric bond cleavage and formation reactions to challenging catalytic processes such as C–H bond functionalization. Our lab recently developed new transition-metal complexes capable of promoting multi-electron reactions, which suggests that a strategy for catalytic alkane functionalization may be attainable. REU Fellows will explore two disparate areas, non-innocent ligands and organometallic chemistry, now being synthesized to develop new catalytic complexes. To incorporate stereo-electronic factors governing reactivity in reaction design, the program interrogates electronic structure using physical-inorganic techniques. Intermingling synthetic and physical methods is central to the program and to training students. REU Fellows will gain exposure to widely-varied techniques for synthesis and characterization of air- and moisture-sensitive transition metal complexes, including NMR and EPR spectroscopies and X-ray crystallography, and to physical methods for elaborating electronic structure, including magnetic susceptibility and electronic spectroscopy. Although relatively nascent, the Heyduk laboratory can count several former undergraduates in the ranks of Ph.D. programs, and typically includes 2-3 undergraduate researchers.

Wilson Ho, Donald Bren Professor, Chemistry, Physics & Astronomy: ***Surface Chemistry***. Probing single molecules on solid surfaces, a new approach to understanding chemical interactions uses a low-temperature scanning tunneling microscope (STM) to image, spectroscopically characterize, manipulate, and chemically modify individual molecules and their interactions with surrounding molecules and environment. Changes in the electronic, vibrational, and spin-dependent spectra reveal the spatial dependence in three dimensions of the chemical interactions between two reactants, providing understanding and control of chemistry at the atomic scale. By combining femtosecond lasers with the STM, time dependent phenomena, such as molecular transformations and spin coherence, can be probed with joint spatial and temporal resolutions. Using ultrahigh vacuum conditions and surface science methodologies to probe organic and inorganic molecules on metal and oxide surfaces, students will be exposed to both physical and chemical techniques. Collaboration will be sought with other REU program chemists to synthesize molecules tailored to specific functions. Besides gaining fundamental understanding, these studies are expected to lead to technological innovations in molecular electronics, catalysis, solar energy conversion, corrosion, and quantum information science. Professor Ho has mentored several REU students during each of the past summers and occasionally during the academic years.

Allon Hochbaum, Associate Professor, Chemistry; Materials Science and Engineering; Chemical and Biomolecular Engineering; Molecular Biology and Biochemistry: ***Rapid Metabolic Fingerprinting of Bacteria for Antibiotic Susceptibility Testing and Environmental Sensors***. The metabolic states of bacteria change quickly and sensitively in response to variations in their local chemical environment. These metabolic shifts can be rapidly assessed with high-throughput spectroscopic methods, in contrast to slower, conventional metabolomic techniques such as mass spectrometry and NMR. In the Hochbaum lab, we use several spectroscopic methods - fluorescence, surface-enhanced Raman, and fluorescence lifetime imaging microscopy - to turn bacteria into living sensors of their environment [*Bhattacharjee et al.*, 2017; *C Q Nguyen et al.*, 2018; *Thrift et al.*, 2017]. These techniques represent a range of rapid sensing platforms for antibiotic susceptibility testing, detection of environmental toxins and heavy metals, and compositional variations of growth media formulations for on-line monitoring of biotechnology processes. REU students in the Hochbaum lab will exploit a subset of these spectroscopic methods to develop new bacterial sensing modalities. Students will develop skills in bacterial culture, spectroscopy and imaging techniques, mass spectrometry, and will have the opportunity to work with liquid handling robots for the automation of high-throughput processes. Since 2012 over 30 undergraduate researchers have worked in the Hochbaum lab (5 currently), continuing on to graduate schools (CU-Boulder, Caltech, USC, UCSD), post-bac research positions (Fulbright Scholarship, Cedars-Sinai Medical Center), and industry (Chevron Phillips, NASA-Jet Propulsion Lab, Johnson & Johnson).

Elizabeth Jarvo, Professor, Chemistry [*Johnson et al.*, 2015; *Kohn et al.*, 2013]: ***Stereoselective Cross-Coupling Reactions for Synthesis of Anti-Cancer Compounds.*** The Jarvo group is developing nickel-catalyzed cross-coupling reactions of alkyl ethers and esters as a new method for enantioselective synthesis, which is a particularly effective method for synthesis of a pharmacophore that is present in compounds with anti-cancer, anti-diabetes, and anti-viral activity. Alkyl ethers are typically not considered reactive electrophiles, however, in the presence of the appropriate catalyst, they undergo coupling with Grignard and organozinc reagents, as well as intramolecular cross-electrophile coupling reactions. Reactions are typically highly stereospecific, where enantioenriched starting material is transformed to enantioenriched product with inversion at the reactive center and high stereochemical fidelity. These methods are particularly effective for synthesis of 1,1-diarylalkanes and substituted cyclopropanes, pharmacophores with activity against a range of biological targets. The REU student will participate by synthesizing new enantioenriched ethers and esters, developing methods for cross-coupling and cross-electrophile coupling reactions, and synthesizing compounds with potential anti-cancer and anti-microbial activity.

Matt Law, Professor, Chemistry, Materials Science and Engineering, Chemical and Biomolecular Engineering [*Y Liu et al.*, 2011; *Zarghami et al.*, 2010]: ***New Materials for Making Green Hydrogen from Water and Sunlight.*** The Law group develops solar energy conversion and storage devices built from nanoscale materials, integrating materials synthesis and fundamental opto-electronic characterization with device fabrication, testing, modeling and optimization. The REU student will synthesize and characterize new nanostructured oxide thin-films or hole-conducting mesoporous materials for a water oxidation half-cell (the side of a water splitting photocell that produces O_2). Molecular ink, hydrothermal and polymeric precursor synthetic techniques will be used to make the films and nanocrystals. Spectroelectrochemistry, impedance measurements, and time-resolved spectroscopy are then applied to determine the band edge energies and flatband potentials of these nanocrystals and to study hole injection and transport in nanocrystalline films. Insights from these fundamental spectroscopic and electronic investigations will be leveraged to build the first efficient, stable, and economical p-type dye photocell that produces O_2 from sunlight. This cell will then be paired with an H_2-evolving cell to split water. Undergraduates from the Law group have been very successful, with many entering graduate school at some of the best institutions (UCB, Northwestern, UCLA). In the past ten years, the Law group has trained 25 undergraduate researchers, most of whom were members of the group for over a year.

Andrej Luptak, Professor, Chemistry, Pharmaceutical Sciences, and Molecular Biology and Biochemistry: ***Discovery of Functional RNAs***. We use a variety of approaches to discover and characterize catalytic RNAs (ribozymes) and highly specific target binders (aptamers). We have implemented both structure–based bioinformatic searches and in vitro selections to uncover functional RNAs. As part of the effort, we have discovered new classes of genomic ribozymes and aptamers. This work, and subsequent characterization of the newly discovered RNAs has greatly benefited from work by undergraduate researchers [*Passalacqua et al.*, 2017; *M M K Vu et al.*, 2012]. We also develop novel methods for more efficient discovery and characterization of functional RNAs, with significant recent contributions by undergraduate researchers [*Chizzolini et al.*, 2020; *Passalacqua et al.*, 2020]. Future REU Fellows will continue to work in this area, with focus on photoactive RNAs and characterization of paradigmatic reactions related to the origin of life on Earth.

Stephen Mang, Assistant Professor of Teaching, Chemistry: ***Incorporating Research Experiences into the Undergraduate Curriculum***. Since the main focus of Dr. Mang's career has been teaching upper-division chemistry laboratory classes, his research interests have evolved to support that focus by developing new experiments [*Harmon et al.*, 2010; *Mang et al.*, 2009] and modifying or creating laboratory courses. Dr. Mang has adapted the curricula of several lab classes to incorporate research experiences, including instrument construction, student-proposed projects, and presentation skills. He has also mentored undergraduates as they developed experiments to be incorporated into the chemistry lab curriculum, in their own classes and in lower-division classes. During the Chem-SURF program Dr. Mang will be directly working with select REU students interested in expanding their research projects into educational activities.

Craig Martens, Professor, Chemistry: ***Molecular Dynamics Simulations of Separation and Purification of Aqueous Solutions***. Students use NAMD software for molecular dynamics simulation to investigate the properties of water around solute species and in nanoenvironments, in systems including aqueous salt solutions in nanopores and clathrate hydrates. The influence of nanometer-scale structure on the solution's boundaries and properties is evaluated by calculating structural and dynamical quantities, such as hydrogen bond lifetimes and correlation functions, versus those of bulk solutions. The free, user-friendly and well supported, NAMD software offers undergraduate students a relatively painless entrée into computational chemistry. A significant UCI NAMD user community of chemists, physicists, and biologists is available for interaction with the student researcher. In addition, close connection with experimental groups at UCI studying the chemistry and physics of water is possible. This fundamental research on water at the nanoscale has applications to nanotechnological approaches to separation and transport of species in aqueous solutions, and to desalination and purification of water. The Martens laboratory has trained a large number of undergraduate researchers.

Rachel Martin, Professor, Chemistry and Molecular Biology & Biochemistry [*Brubaker et al.*, 2011; *Butts et al.*, 2016a; *Butts et al.*, 2016b; *Unhelkar et al.*, 2017]: ***From Genomic Source Code to Enzyme Discovery in Carnivorous Plants***. With the advent of inexpensive gene sequencing, genomic data proliferates at a pace that far outstrips experimental resources for protein characterization. The overall goal of this project is to provide a road map for approaching complex systems of biomolecules in which many similar isoforms are employed simultaneously. The first target is *Drosera capensis*, a carnivorous plant that catches its prey using flypaper traps. Carnivorous plants face unique proteomic challenges and are thus a potentially valuable resource for the discovery of enzymes with improved or novel functional characteristics. Participating REU students will be introduced to bioinformatics tools, molecular modeling, protein expression and purification, and/or functional enzyme characterization. Undergraduates start by preparing proteins and performing bioinformatics analyses under close supervision from their graduate student mentors and gradually become more independent as they build their skills. By the time they graduate, our most motivated undergraduates are already performing at the level expected of first-year Ph.D. students. Professor Martin has mentored more than 50 undergraduates from chemistry, biology, and engineering. Most of her alumni have moved on to Ph.D. programs and several received NSF GRFP fellowships.

David Mobley, Associate Professor, Chemistry and Pharmaceutical Sciences [*Bannan et al.*, 2016; *Duarte Ramos Matos et al.*, 2017; *S Liu et al.*, 2016; *Mobley et al.*, 2014]: ***Protein-ligand Interactions, Solvation, and Solubility***. The Mobley group works on developing, testing, and applying computational techniques to help aid pharmaceutical drug discovery. They have major interests in predicting protein-ligand binding, as well as solvation properties and solubilities of small drug-like molecules. Students in the group work on a range of projects, including high-throughput studies of binding (such as with docking techniques), detailed binding free energy calculations using molecular dynamics simulations, and studies of solvation or energetics of small molecules in the gas phase or in solution. Interested students are involved with projects like the Statistical Assessment of the Modeling of Proteins and Ligands (SAMPL) series of challenges, where they run community blind prediction challenges to test the state of computational methods in the field. Usually projects have implications relating to pharmaceutical drug discovery, either directly or by helping to improve the predictive power of their tools. The work is entirely computational, but the group members often collaborate with experimental groups. Professor Mobley has mentored 20 undergraduate students, and many of them have published work done in the group.

Craig Murray, Associate Professor, Chemistry [*Elizabeth S. Foreman et al.*, 2015; *E. S. Foreman et al.*, 2016; *Tadayon et al.*, 2018]: ***Kinetics and reactivity of Criegee intermediates.*** Ozonolysis of alkenes is an important reaction in the atmosphere and leads to the formation of carbonyl oxides, known as Criegee intermediates (CIs). Reactions of stabilized CIs with other gases found in the atmosphere have been suggested to lead to particle formation, which can impact air quality, health, and ultimately climate. Understanding CI reactivity is a critical first step to assessing their role in atmospheric chemistry. The project involves the use laser flash photolysis and transient absorption spectroscopy in a flow reactor to study the kinetics of reactions between Criegee intermediates and atmospheric trace gases. The REU student will learn how to perform the experimental measurements and analyze and interpret the data acquired. Dr. Murray has mentored 13 undergraduate students in his laboratory, many of whom have co-authored publications and advanced to graduate programs.

Sergey Nizkorodov, Professor, Chemistry [*Aiona et al.*, 2017; *Epstein et al.*, 2012; *Hinks et al.*, 2016; *Hinks et al.*, 2018; *Lignell et al.*, 2013; *MacMillan et al.*, 2012; *Malecha et al.*, 2018; *T B Nguyen et al.*, 2012; *D. E. Romonosky et al.*, 2016; *Dian E. Romonosky et al.*, 2015; *Tran et al.*, 2017; *Updyke et al.*, 2012]: ***Chemistry of Organic Aerosols***. A significant fraction of volatile organic air pollutants emitted by traffic and industrial sources are converted into fine particles. This organic aerosol contributes to visibility degradation, reduces the air quality in urban areas, and affects regional climate. Light-absorbing "black" and "brown" particles are of particular concern as they heat up the air by absorbing solar radiation. To determine what compounds are responsible for the brown aerosol in urban air, the research group investigates detailed composition and chemical properties of organic aerosols produced from various anthropogenic air pollutants. The aerosols are generated by photochemical oxidation of selected volatile organic precursors in the UCI smog chamber or flow tubes equipped with a host of state-of-the art instruments. The REU participant will be given a compressed course in atmospheric and aerosol chemistry, and standard atmospheric chemistry measurement methods. The REU participant will learn to prepare various types of aerosols using smog chamber and flow tube methods, characterize optical properties of the aerosol, and analyze aerosol composition by mass spectrometry, and other analytical methods. Over 40 students, including summer researchers, have done research in the Nizkorodov Lab, and many won prestigious awards, contributed to writing peer-reviewed publications, and went to graduate or professional schools.

James Nowick, Professor, Chemistry [*Chen et al.*, 2017a; *Chen et al.*, 2017b; *Ferrick et al.*, 2015; *Kreutzer et al.*, 2016; *Kreutzer et al.*, 2017; *Salveson et al.*, 2018; *Wang et al.*, 2018; *Yang et al.*, 2017]: ***Supramolecular Chemistry of Amyloidogenic Peptides***. This project seeks to learn more about the structures of amyloid oligomers through the use of chemical models systems. Amyloid oligomers appear to be the toxic agents responsible for neurodegeneration and cellular death in amyloid diseases such as Alzheimer's disease, frontotemporal dementias, Parkinson's disease, and type 2 diabetes. Relatively little is known about the structures of amyloid oligomers, and only a few studies have provided glimpses of amyloid oligomers at atomic resolution. Dr. Nowick and his students have developed an effective strategy to elucidate the structures of oligomers formed by amyloidogenic peptides: incorporating the peptides into macrocycles and using a single N-methyl group to prevent uncontrolled aggregation to fibrils. The resulting macrocyclic beta-sheet peptides assemble to form well-defined oligomers, and a good fraction of the peptides form crystals suitable for X-ray crystallography. Students are using this approach to elucidate the structures of oligomers from amyloidogenic peptides derived from the protein tau, the protein alpha-synuclein, and the islet amyloid polypeptide (IAPP, amylin). The structures of the oligomers that form are determined at atomic resolution by X-ray crystallography, and the crystallographic structures of the oligomers are correlated with the solution state biological and biophysical properties. Professor Nowick has mentored 60 undergraduate students. A number of undergraduates have coauthored papers that have been published or submitted, and have gone on to graduate schools in Chemistry.

Reginald Penner, Chancellor's Professor, Chemistry: ***Polymer Nanowire Growth Using Electrochemical Step Edge****.* Lithographically patterned Nanowire Electrodeposition (LPNE) is a new method for the patterning ultra-long (millimeters) nanowires of metals and semiconductors on dielectrics like glass and plastics. We are studying the application of the nanowire obtained using the LPNE method to the preparation of new types of chemical sensors, optical detectors, and a variety of other devices. Professor Penner has supervised 10 local Irvine high school students over the last six years: eight have gone on to graduate schools (UC Berkeley, MIT, Dartmouth College, Caltech, Harvard,), and two are presently in the group. In addition, a large number of undergraduates have trainedin the Penner laboratory.

Eric Potma, Professor, Chemistry and Beckman Laser Institute [*Gallagher et al.*, 2015; *Hanninen et al.*, 2017; *Kenison et al.*, 2017]: ***Molecular Orientation and Crosslinking in Collagen Fibers.*** The Potma group focuses on investigating molecular distribution and molecular orientation in complex natural materials such as cellulose fibers, keratin fibers and collagen, using a suite of spectroscopic imaging techniques based on vibrational contrast. His research tools consist of a suite of spectroscopic imaging techniques based on vibrational contrast, including Fourier-transform infrared (FTIR) spectroscopy, Raman microscopy, and sum-frequency generation (SFG) microscopy. The REU project will focus on the molecular orientation of collagen fibrils in tissues. The REU student will perform SFG microscopy of several collagen-rich samples and help determine the orientation and crosslinking of the fibers. The SFG instrumentation is rather challenging for most students. Our experience indicates, however, that once students have received an extensive training on this instrument, most trainees feel empowered and confident to take on challenging imaging experiments. After the REU student has acquired sufficient training, the student will have the opportunity to independently design and schedule measurements. Since his arrival at UCI in 2005, Professor Potma has mentored over 30 undergraduate students in his laboratory. Importantly, the number of undergraduate students has increased over time, with 2 to 4 undergraduate researchers working in the laboratory at any given time.

Jennifer Prescher, Professor, Chemistry and Molecular Biology & Biochemistry [*M D Liu et al.*, 2018; *Rathbun et al.*, 2017; *Rachel C. Steinhardt et al.*, 2016; *R. C. Steinhardt et al.*, 2017]: ***Generating Orthogonal Bioluminescent Probes for Multi-cellular Imaging in Vivo***. Bioluminescence imaging is among the most powerful techniques for visualizing cells in complex tissues and organisms. At the core of this technology are enzymes (luciferases) that catalyze the oxidation of small molecule substrates (luciferins) to release visible light. Several luciferase-luciferin pairs exist in nature, and many have been adapted for tracking cells and gene expression patterns in whole animals. Unfortunately, the optimal luciferases for *in vivo* imaging utilize the same substrate, and therefore cannot be used to distinguish multiple cell types in a single subject. The Prescher group members are expanding the bioluminescence toolkit by creating new luciferases that are responsive to unique luciferin substrates (i.e., "orthogonal" pairs). Their approach involves re-engineering firefly luciferase, generating a panel of mutant enzymes that accept chemically distinct luciferin analogs. When the mutants and analogs are mixed together, light is produced when complementary enzyme-substrate partners interact. The REU participants will be involved in diverse aspects of this project, including chemical syntheses and enzyme engineering. Such studies will provide some of the first macroscopic images of tumor heterogeneity, immune function, and other complex networks, and may fundamentally change existing views on human health and disease. Additionally, the bioluminescent probes will likely inspire new discoveries in a broad spectrum of fields. More than 20 undergraduates, including summer students, have contributed to the ongoing research program in the Prescher group. Many of them have contributed to publications, been recognized by external awards, or continued on to graduate or other professional training.

Scott Rychnovsky, Professor, Chemistry [*A. S. Burns et al.*, 2018; *Alexander S. Burns et al.*, 2017; *Miller et al.*, 2012; *Samame et al.*, 2016; *Tay et al.*, 2014; *Wagner et al.*, 2011; *Wagner et al.*, 2016; *Wagner et al.*, 2014]: ***Designing Cleavable Cross-linkers to Map Protein-Protein***

interactions. In collaboration with Professor Lan Huang's group, we have been developing new protein cross-linkers that cleave in the Mass Spectrometer. CID (collision-induced dissociation) facilitates the sequencing of the peptide chains and allows the sites of cross-linking to be identified and mapped. We design small molecules to interact selectively with the various amino acid side chains. Chemical enrichment through click reactions is also desirable. The project in my lab focuses on the synthesis of these target molecules using organic synthesis. The proteomics aspect of the project is done in the Huang lab, but we interact closely on this project. The project provides good training in organic synthesis and a simple introduction to proteomics.

Eric Saltzman, Professor, Chemistry and ESS. ***Ice core studies of atmospheric trace gases.*** The bubbles in polar ice cores contain an amazing archive recording the history of atmospheric composition. Our laboratory extracts and analyzes air from ice cores from Greenland and Antarctica in order to study the history of trace gases and how they are influenced by climate change. Student projects involve investigating the biogeochemical cycles of various trace gases, analyzing ice core data, and using simple computer simulations to explain changes in the atmospheric abundance of trace gases in the past.

Kenneth Shea, Professor, Chemistry, Chemical Engineering and Material Science: ***Tunable Optical and Mechanical Properties of Polymers and Materials***. Polymers and materials, many of which are "one of a kind," enable the researcher to acquire a broad range of characterization skills. One project involves polymers and materials with "tunable" optical and mechanical properties and would expose the student to small-molecule, polymer, and materials synthesis, and a variety of characterization techniques. Historically, undergraduate students on these summer projects wind up as coauthors on publications. Bridged polysilsesquioxanes are fabricated from molecular building blocks composed of a variable organic component and two or more sol-gel polymerizable trialkoxy silanes. Important physical characteristics include high surface area, pore volume, and functional group loading. One project, involving photo-responsive materials, is synthesizing bifunctional coumarin photodimers, monomers incorporated into the backbone of materials ranging from elastermers to thermosets, which include silicone linear polymers and networks and bridged polysilsesquioxanes. We are evaluating these materials' optical and mechanical properties before and after short wavelength and UV irradiation using fluorescence microscopy, AFM, imaging ellipisometry, gas absorption (SA analysis), and solid-state NMR. The materials have applications in waveguide fabrication and secure encryption, and as UV dosimeters. Professor Shea has served as mentor for over 60 undergraduates. Almost all of these students have gone on to graduate or professional school. These students now occupy positions in academics government laboratories and industry. In addition a significant number have gone on to medical school to become doctors. Over the span of his career they have been coauthors of over sixteen manuscripts and they have presented numerous papers at scientific meetings and conferences.

Manabu Shiraiwa, Associate Professor, Chemistry: ***Kinetic modeling of organic aerosol chemistry or experimental studies of reactive oxygen species (ROS) and radicals in atmospheric fine particulate matter***. Organic manic aerosols and ROS play a central role in aerosol effects on air quality, climate, and public health. There are two possible projects for a REU participant: 1) kinetic multilayer modeling of gas-particle interactions and aerosol chemistry (remote); 2) quantification of ROS associated with aerosol particles using an electron paramagnetic resonance (EPR) spectrometer (onsite). Participants will work with the PI, graduate students or postdoctoral fellows in the group, and participate in weekly group meetings.

Seu Sim, Assistant Professor, Chemistry; Biomedical Engineering; Chemical and Biomolecular Engineering: ***Engineering and understanding cell-material interface***. The Sim laboratory is interested in research problems at the interface of chemistry, bioengineering, and materials science and expanding our limited knowledge of the cell-material interface. Our goal is to develop novel 3D-printable biomaterials where living cells' functionalities are integrated into synthetic polymeric scaffolds. REU participants will perform polymer synthesis, molecular cloning, protein expression/purification, depending on their prior experience and research interest. By participating in this REU program, students will learn key characterization methods in soft materials chemistry and/or molecular biology.

Zuzanna Siwy, Professor, Physics and Chemistry [*Innes et al.*, 2010; *Pevarnik et al.*, 2012; *Powell et al.*, 2008; *Qiu et al.*, 2015]: ***Preparation of biomimetic nanopores and ionic circuits***. Ion transport through channels and pores embedded in a cell membrane is the basis of all physiological processes of a living organism. In this project, the REU participant will learn fabrication of single nanopores whose transport properties resemble these of biological channels. For example, voltage gated channels open and close in response to electric field. The project will also involve chemical modification of the pore walls, microscopy and electrochemical characterization. The REU participant will also create an ionic circuit consisting of two pores with different functionalities.

Jim Smith, Professor, Chemistry: ***Investigations of atmospheric new particle formation and growth***. In this project, the REU participant will team with graduate students on laboratory and field measurements focusing on the formation and growth of atmospheric aerosol particles. Our laboratory has developed novel instruments to study the composition of the smallest particles in the atmosphere, with diameters as small as 5 nm, as well as the gases that are responsible for the new particle formation and growth. Our current lab studies address questions such as "What possible roles do organic compounds play in the formation of the stable clusters and for the growth of these clusters into new particles?" and "Are the compounds responsible for the birth and growth of atmospheric aerosol particles formed in the atmosphere or within the particles themselves? Prof. Smith has mentored several undergraduates in his lab - an average of 3 per quarter/summer. Undergraduates contribute to research that address everyday environmental challenges including air pollution and climate change. There are also opportunities for undergraduates to learn about the instruments used in atmospheric research and contribute to instrument development efforts in the lab.

> Specific to 2021: ***Design and resting of masks for COVID-19 mitigation***. In this project, the REU student will team with Prof. Smith and his graduate students in testing different materials and designs that are being employed for respiratory protection during the current COVID-19 pandemic. This project is part of a larger effort called the UCI Face Mask Project (https://sites.uci.edu/ucimask/). To assist us in this task, we have developed a mannequin-based testing facility that not only allows us to measure mask filtration efficiency but also the effects caused by improperly fitted masks. Students will learn about the instruments that we use to size and count aerosol particles, with applications that extend to the sizing of atmospheric aerosol particles

Douglas Tobias, Professor and Department Chair, Chemistry [*Brubaker et al.*, 2011; *Kyrychenko et al.*, 2018; *Schow et al.*, 2012]: ***Toward Molecular-Scale Models of Congenital and Age-Related Cataract: Molecular Modeling Studies of Structural Proteins in the Eye Lens.*** The eye lens elongated fiber cells contain a high-concentration solution of crystallin proteins, and precipitation of crystallins leads to cataract, a major cause of blindness worldwide. The REU student will carry out atomistic molecular dynamics (MD) simulations that will elucidate protein-protein interactions in solutions of wild-type crystallins and their cataract-related variants that will contribute to the development of atomically detailed structural models of individual crystallin molecules and their organization in soluble and aggregated states. Specifically, MD simulations of single molecules of wild type, congenital cataract-related mutants, and de-amidated variants of gamma S-crystallin will be used to gain insights into the changes in structural dynamics and hydration that result from modifications of the protein sequence, and validated by comparison with experimental data, in collaboration with Professor Rachel Martin. Configurations from the MD simulations will be used as input into Monte Carlo simulations of concentrated solutions of wild-type and cataract-prone crystallins that will provide molecular-scale insight into the role of altered protein-protein interactions in crystallin aggregation. By participating in this project, the student will be trained in state-of-the-art computer simulation techniques, computer programming, and molecular graphics, and will have the opportunity to work in close collaboration with experimental biophysicists and structural biologists. Professor Tobias has mentored over 20 undergraduate students in research. All of the REU alumni from the Tobias group have ended up in top-notch M.D., M.D./Ph.D., and chemistry graduate programs, several are co-authors on publications, and a few have been awarded prestigious fellowships.

Shiou-Chuan (Sheryl) Tsai, Professor, Chemistry; Molecular Biology and Biochemistry; Pharmaceutical Sciences: ***Chemical Biology and Structural Enzymology of Natural Product Biosynthesis***. The Tsai lab investigates the chemical biology and structural biology of enzymes that biosynthesize natural products, which include many pharmaceutically important compounds. This project aims to determine the molecular basis of substrate specificity of three enzyme complexes that biosynthesize pharmaceutically active polyketides: acyl-CoA carboxylase (ACCase), polyketide synthase (PKS), and deoxysugar-synthesizing enzymes. The long-term goal is to biosynthesize new "unnatural" natural products and screen them for pharmaceutical activity. The central hypothesis is that the product from these three complexes can be changed by mutating active site residues of ACCase, PKS, and sugar-synthesizing enzymes. REU Fellows will be exposed to such techniques as identification of active site residues by site-directed mutagenesis; probes of the PKS active site by solving PKS crystal structures, and probes of enzyme active sites by biophysical methods. Problem-based learning will emphasize strategic polyketide metabolism concepts and structure-function relationships across genomes of organisms that produce polyketides. Professor Tsai has mentored 60+ undergraduates during the past seven years. Many of these students are now in graduate school or have completed graduate school.

Christopher Vanderwal, Professor, Chemistry: ***Synthesis of Natural Products***. Our lab seeks to find innovative strategies for the efficient synthesis of complex, bioactive natural products. The prospective REU student will be paired with a graduate student mentor and will learn how to plan and execute multi-step chemical syntheses. This project is ideal for an undergraduate research participant, as he/she will be exposed to a variety of organic chemical reactions and related techniques, including structural assignments via NMR and mass spectrometry. Weekly research and literature group meetings, in addition to formal and informal mentoring sessions with the advisor, will greatly enhance the REU experience.

David Van Vranken, Professor, Chemistry [*Arredondo et al.*, 2017; *Gutman et al.*, 2014; *Kitamura et al.*, 2015; *Premachandra et al.*, 2015]: ***Integration of Machine Learning with Organic Synthesis***. Organic chemists design and synthesize the types of molecules that drive modern society like powerful new medicines, functional materials, and biological probes. The reactions that are developed and used by synthetic organic chemists are imprecise, generating mixtures of the anticipated products and inscrutable side products. The Van Vranken group is exploiting machine learning to identify the molecular debris that is omnipresent in synthetic organic reactions, drug degradation processes, and other chemical processes. The group develops novel palladium-catalyzed reactions of carbene groups to assemble structurally complex organic molecules. REU students will learn traditional techniques of organic synthesis including inert atmosphere reaction techniques, chromatographic purification of products and spectroscopic characterization. The Van Vranken group has mentored 28 undergraduate researchers (three current), and have a strong track record of having undergraduates publish their work.

Gregory Weiss, Professor, Chemistry and Molecular Biology and Biochemistry [*Choi et al.*, 2013; *Gilliam et al.*, 2016; *Ogata et al.*, 2017; *Yuan et al.*, 2015]: ***Listening to Individual Molecules and Cancer Biomarkers with Nanotechnology***. Dr. Weiss' lab develops new tools to dissect the relationship between protein structure and function. Many projects apply phage display to access vast libraries of bacteriophage-presented peptides and proteins. The Weiss lab has identified binding partners to cancer-associated biomarkers, including prostate tumor antigens (PSMA and PSA). The resultant phage with the cancer-binders have been wired into nanometer-scale electrical circuits for direct measurement of cancer marker levels in the early diagnosis of cancer [*Ogata et al.*, 2017]. He has extended a similar bioelectronic system to an individual enzyme molecule wired into electronic circuits based on carbon nanotubes; recent studies focus on two cancer-associated enzymes and therapeutic targets, cAMP-dependent Protein Kinase A and DNA polymerase [*Choi et al.*, 2013]. Professor Weiss has trained more than 45 undergraduate researchers, including 4-6 undergraduates every quarter for the last three years. Seven undergraduates have co-authored four publications from the lab during this period [*Choi et al.*, 2013; *Gilliam et al.*, 2016; *Ogata et al.*, 2017; *Yuan et al.*, 2015], and two undergraduates were part of the team awarded an Ig Nobel Prize for "partially unboiling an egg" [*Yuan et al.*, 2015]. The majority of undergraduates who have graduated from the Weiss lab have pursued science careers, including PhD programs at UCSF, U. Wisconsin, U. North Carolina, City of Hope, and other institutions.

Jenny Yang, Associate Professor, Chemistry [*Hanna et al.*, 2019; *Kotyk et al.*, 2018; *Lydon et al.*, 2016; *Shaffer et al.*, 2016; *N. Sutthirat et al.*, 2018; *Natwara Sutthirat et al.*, 2019; *Thammavongsy et al.*, 2016; *Tsay et al.*, 2015]: ***Inorganic Synthesis, Small Molecule Catalysis, Solar Fuels***. The research efforts in Dr. Yang's group are focused on the development of catalysts for the production and utilization of carbon-neutral chemical fuels from renewable energy sources. Undergraduate researchers will learn how to synthesize and characterize new ligands and metal complexes using air-sensitive techniques. They will also learn how to characterize catalytic activity using electrochemical methods. Detailed mechanistic and kinetic studies will complement the electrochemical studies to achieve insights into improving catalyst design. REU Fellows will work on independent projects with the goal of publishing their work. They will work with the PI and with other graduate students or postdoctoral fellows in the group, and participate in weekly sub-group and super-group meetings, as well as literature reviews. Since 2013, Professor Yang has mentored 21 undergraduate researchers. Of those who have completed their degree (16), all have gone on to graduate programs or industrial positions in a

STEM area. Five of those students have completed research for their Honors thesis in her lab and eleven have also been co-authors on ten different peer-reviewed publications.

Selected Papers by the Faculty Mentors (Most Published with Undergraduate Researchers)

Aiona, P. K., H. J. Lee, R. Leslie, P. Lin, A. Laskin, J. Laskin, and S. A. Nizkorodov (2017), Photochemistry of Products of the Aqueous Reaction of Methylglyoxal with Ammonium Sulfate, *ACS Earth Space Chem.*, *1*(8), 522-532, doi:10.1021/acsearthspacechem.7b00075.

Arredondo, V., S. C. Hiew, E. S. Gutman, I. Premachandra, and D. L. Van Vranken (2017), Enantioselective Palladium-Catalyzed Carbene Insertion into the N-H Bonds of Aromatic Heterocycles, *Angewandte Chemie-International Edition*, *56*(15), 4156-4159, doi:10.1002/anie.201611845.

Bannan, C. C., G. Calabro, D. Y. Kyu, and D. L. Mobley (2016), Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water, *Journal of Chemical Theory and Computation*, *12*(8), 4015-4024, doi:10.1021/acs.jctc.6b00449.

Bhattacharjee, A., R. Datta, E. Gratton, and A. I. Hochbaum (2017), Metabolic fingerprinting of bacteria by fluorescence lifetime imaging microscopy, *Scientific Reports*, *7*(1), 3743, doi:10.1038/s41598-017-04032-w.

Brubaker, W. D., J. A. Freites, K. J. Golchert, R. A. Shapiro, V. Morikis, D. J. Tobias, and R. W. Martin (2011), Separating Instability from Aggregation Propensity in gamma S-Crystallin Variants, *Biophysical Journal*, *100*(2), 498-506, doi:10.1016/j.bpj.2010.12.3691.

Burns, A. S., C. C. Ross, and S. D. Rychnovsky (2018), Heteroatom-Directed Acylation of Secondary Alcohols To Assign Absolute Configuration, *Journal of Organic Chemistry*, *83*(5), 2504-2515, doi:10.1021/acs.joc.7b03156.

Burns, A. S., A. J. Wagner, J. L. Fulton, K. Young, A. Zakarian, and S. D. Rychnovsky (2017), Determination of the Absolute Configuration of β-Chiral Primary Alcohols Using the Competing Enantioselective Conversion Method, *Organic Letters*, *19*(11), 2953-2956, doi:10.1021/acs.orglett.7b01189.

Butts, C. T., J. C. Bierma, and R. W. Martin (2016a), Novel proteases from the genome of the carnivorous plant Drosera capensis: Structural prediction and comparative analysis, *Proteins-Structure Function and Bioinformatics*, *84*(10), 1517-1533, doi:10.1002/prot.25095.

Butts, C. T., X. H. Zhang, J. E. Kelly, K. W. Roskamp, M. H. Unhelkar, J. A. Freites, S. Tahir, and R. W. Martin (2016b), Sequence comparison, molecular modeling, and network analysis predict structural diversity in cysteine proteases from the Cape sundew, Drosera capensis, *Computational and Structural Biotechnology Journal*, *14*, 271-282, doi:10.1016/j.csbj.2016.05.003.

Cardon, J. M., G. Krueper, R. Kautz, D. M. Fabian, J. Angsono, H. Chen, and S. Ardo (2020), Reconciliation of differences in apparent diffusion coefficients measured for self-exchange electron transfer between molecules anchored to mesoporous titanium dioxide thin films, *ACS Applied Materials & Interfaces*, DOI: 10.1021/acsami.1029b19096.

Carlton, A. G., A. E. Christiansen, M. M. Flesch, C. J. Hennigan, and N. Sareen (2020), Mulitphase Atmospheric Chemistry in Liquid Water: Impacts and Controllability of Organic Aerosol, *Acc. Chem. Res.*, *53*(9), 1715-1723, doi:10.1021/acs.accounts.0c00301.

Carlton, A. G., E. Little, M. Moeller, S. Odoyo, and P. B. Shepson (2014), The Data Gap: Can a Lack of Monitors Obscure Loss of Clean Air Act Benefits in Fracking Areas?, *Environ. Sci. Technol.*, *48*(2), 893-894, doi:10.1021/es405672t.

Chen, K. H., K. A. Corro, S. P. Le, and J. S. Nowick (2017a), X-ray Crystallographic Structure of a Giant Double-Walled Peptide Nanotube Formed by a Macrocyclic beta-Sheet Containing A beta(16-22), *J. Amer. Chem. Soc.*, *139*(24), 8102-8105, doi:10.1021/jacs.7b03890.
Chen, K. H., S. P. Le, X. Han, J. M. Frias, and J. S. Nowick (2017b), Alanine scan reveals modifiable residues in teixobactin, *Chemical Communications*, *53*(82), 11357-11359, doi:10.1039/c7cc03415f.
Chizzolini, F., L. F. M. Passalacqua, M. Oumais, A. I. Dingilian, J. W. Szostak, and A. Luptak (2020), Large Phenotypic Enhancement of Structured Random RNA Pools, *J. Amer. Chem. Soc.*, *142*(4), 1941-1951, doi:10.1021/jacs.9b11396.
Choi, Y., T. J. Olsen, P. C. Sims, I. S. Moody, B. L. Corso, M. N. Dang, G. A. Weiss, and P. G. Collins (2013), Dissecting Single-Molecule Signal Transduction in Carbon Nanotube Circuits with Protein Engineering, *Nano Letters*, *13*(2), 625-631, doi:10.1021/nl304209p.
Cruz, F. A., Z. W. Chen, S. I. Kurtoic, and V. M. Dong (2016), Tandem Rh-catalysis: decarboxylative beta-keto acid and alkyne cross-coupling, *Chemical Communications*, *52*(34), 5836-5839, doi:10.1039/c6cc02522f.
Cruz, F. A., Y. Zhu, Q. D. Tercenio, Z. Shen, and V. M. Dong (2017), Alkyne Hydroheteroarylation: Enantioselective Coupling of Indoles and Alkynes via Rh-Hydride Catalysis, *J. Amer. Chem. Soc.*, *139*(31), 10641-10644, doi:10.1021/jacs.7b05893.
Duarte Ramos Matos, G., D. Y. Kyu, H. H. Loeffler, J. D. Chodera, M. R. Shirts, and D. L. Mobley (2017), Approaches for Calculating Solvation Free Energies and Enthalpies Demonstrated with an Update of the FreeSolv Database, *Journal of Chemical & Engineering Data*, *62*(5), 1559-1569, doi:10.1021/acs.jced.7b00104.
Epstein, S. A., D. Shemesh, V. T. Tran, S. A. Nizkorodov, and R. B. Gerber (2012), Absorption Spectra and Photolysis of Methyl Peroxide in Liquid and Frozen Water, *J. Phys. Chem. A*, *116*(24), 6068-6077, doi:10.1021/jp211304v.
Ezell, M. J., W. H. Wang, D. Shemesh, A. Ni, R. B. Gerber, and B. J. Finlayson-Pitts (2019), Experimental and Theoretical Studies of the Environmental Sensitivity of the Absorption Spectra and Photochemistry of Nitenpyram and Analogs, *ACS Earth Space Chem.*, *3*(9), 2063-2075, doi:10.1021/acsearthspacechem.9b00179.
Faiola, C. L., et al. (2018), Terpene Composition Complexity Controls Secondary Organic Aerosol Yields from Scots Pine Volatile Emissions, *Scientific Reports*, *8*, doi:10.1038/s41598-018-21045-1.
Faiola, C. L., et al. (2019), Secondary Organic Aerosol Formation from Healthy and Aphid-Stressed Scots Pine Emissions, *ACS Earth Space Chem.*, *3*(9), 1756-1772, doi:10.1021/acsearthspacechem.9b00118.
Ferrick, K., R., N. Truex, and J. S. Nowick (2015), Mimicry and Study of Amyloidogenic Peptides with Macrocyclic β-Sheet Models (paper T41), in *44th National Organic Chemistry Symposium*, edited, p. T41, College Park, MD, United States.
Finkeldei, S., et al. (2017), Composition dependent order-disorder transition in NdxZr1-xO2-0.5x pyrochlores: A combined structural, calorimetric and ab initio modeling study, *Acta Materialia*, *125*, 166-176, doi:10.1016/j.actamat.2016.11.059.
Finkeldei, S., M. C. Stennett, P. M. Kowalski, Y. Ji, E. de Visser-Tynova, N. C. Hyatt, D. Bosbach, and F. Brandt (2020), Insights into the fabrication and structure of plutonium pyrochlores, *Journal of Materials Chemistry A*, *8*(5), 2387-2403, doi:10.1039/c9ta05795a.
Finkeldei, S. C., J. O. Kiggans, R. D. Hunt, A. T. Nelson, and K. A. Terrani (2019), Fabrication of UO2-Mo composite fuel with enhanced thermal conductivity from sol-gel feedstock, *Journal of Nuclear Materials*, *520*, 56-64, doi:10.1016/j.jnucmat.2019.04.011.
Foreman, E. S., K. M. Kapnas, Y. Jou, J. Kalinowski, D. Feng, R. B. Gerber, and C. Murray (2015), High resolution absolute absorption cross sections of the [B with combining tilde]1A[prime or minute]-[X with combining tilde]1A[prime or minute] transition of the CH2OO biradical, *Phys. Chem. Chem. Phys.*, *17*(48), 32539-32546, doi:10.1039/C5CP04977F.

Foreman, E. S., K. M. Kapnas, and C. Murray (2016), Reactions between Criegee Intermediates and the Inorganic Acids HCl and HNO3: Kinetics and Atmospheric Implications, *Angewandte Chemie-International Edition*, *55*(35), 10419-10422, doi:10.1002/anie.201604662.
Freeman, F., I. T. Adesina, J. Le La, J. Y. Lee, and A. A. Poplawski (2013), Conformers of Cysteine and Cysteine Sulfenic Acid and Mechanisms of the Reaction of Cysteine Sulfenic Acid with 5,5-Dimethyl-1,3-cyclohexanedione (Dimedone), *J. Phys. Chem. B*, *117*(50), 16000-16012, doi:10.1021/jp409022m.
Freeman, F., A. Bui, L. Dinh, and W. J. Hehre (2012), Dehydrative Cyclocondensation Mechanisms of Hydrogen Thioperoxide and of Alkanesulfenic Acids, *J. Phys. Chem. A*, *116*(30), 8031-8039, doi:10.1021/jp3024827.
Furche, F., B. T. Krull, B. D. Nguyen, and J. Kwon (2016), Accelerating molecular property calculations with nonorthonormal Krylov space methods, *J. Chem. Phys.*, *144*(17), doi:10.1063/1.4947245.
Gallagher, K. L., A. Alfonso-Garcia, J. Sanchez, E. O. Potma, and G. M. Santos (2015), Plant growth conditions alter phytolith carbon, *Frontiers in Plant Science*, *6*, doi:10.3389/fpls.2015.00753.
Gilliam, A. J. H., J. N. Smith, D. Flather, K. M. Johnston, A. M. Gansmiller, D. A. Fishman, J. M. Edgar, M. Balk, S. Majumdar, and G. A. Weiss (2016), Affinity-Guided Design of Caveolin-1 Ligands for Deoligomerization, *Journal of Medicinal Chemistry*, *59*(8), 4019-4025, doi:10.1021/acs.jmedchem.5b01536.
Gutman, E. S., V. Arredondo, and D. L. Van Vranken (2014), Cyclization of eta(3)-Benzylpalladium Intermediates Derived from Carbene Insertion, *Organic Letters*, *16*(20), 5498-5501, doi:10.1021/ol502813u.
Hanna, C. M., A. Luu, and J. Y. Yang (2019), Proton-Coupled Electron Transfer at Anthraquinone Modified Indium Tin Oxide Electrodes, *ACS Applied Energy Materials*, *2*(1), 59-65, doi:10.1021/acsaem.8b01568.
Hanninen, A., M. W. Shu, and E. O. Potma (2017), Hyperspectral imaging with laser-scanning sum-frequency generation microscopy, *Biomed. Opt. Express*, *8*(9), 4230-4242.
Harmon, C. W., S. A. Mang, J. Greaves, and B. J. Finlayson-Pitts (2010), Identification of fatty acids, phospholipids, and their oxidation products using matrix-assisted laser desorption ionization mass spectrometry and electrospray ionization mass spectrometry, *Journal of Chemical Education*, *87*(2), 186-189.
Hinks, M. L., M. V. Brady, H. Lignell, M. J. Song, J. W. Grayson, A. K. Bertram, P. Lin, A. Laskin, J. Laskin, and S. A. Nizkorodov (2016), Effect of viscosity on photodegradation rates in complex secondary organic aerosol materials, *Phys. Chem. Chem. Phys.*, *18*(13), 8785-8793, doi:10.1039/c5cp05226b.
Hinks, M. L., J. Montoya-Aguilera, L. Ellison, P. Lin, A. Laskin, J. Laskin, M. Shiraiwa, D. Dabdub, and S. A. Nizkorodov (2018), Effect of relative humidity on the composition of secondary organic aerosol from the oxidation of toluene, *Atmos. Chem. Phys.*, *18*(3), 1643-1652, doi:10.5194/acp-18-1643-2018.
Innes, L., M. R. Powell, I. Vlassiouk, C. Martens, and Z. S. Siwy (2010), Precipitation-Induced Voltage-Dependent Ion Current Fluctuations in Conical Nanopores, *Journal of Physical Chemistry C*, *114*(18), 8126-8134, doi:10.1021/jp910815p.
Johansson, M. P., I. Warnke, A. Le, and F. Furche (2014), At What Size Do Neutral Gold Clusters Turn Three-Dimensional?, *Journal of Physical Chemistry C*, *118*(50), 29370-29377, doi:10.1021/jp505776d.
Johnson, A. G., M. M. Tranquilli, M. R. Harris, and E. R. Jarvo (2015), Selective synthesis of either enantiomer of an anti-breast cancer agent via a common enantioenriched intermediate, *Tetrahedron Letters*, *56*(23), 3486-3488, doi:10.1016/j.tetlet.2015.02.121.

Kenison, J. P., A. Fast, F. Guo, A. LeBon, W. Jiang, and E. O. Potma (2017), Imaging properties of surface-enhanced coherent anti-Stokes Raman scattering microscopy on thin gold films, *J. Opt. Soc. Am. B*, *34*(10), 2104-2014.
Kim, D. K., J. Riedel, R. S. Kim, and V. M. Dong (2017), Cobalt Catalysis for Enantioselective Cyclobutanone Construction, *J. Amer. Chem. Soc.*, *139*(30), 10208-10211, doi:10.1021/jacs.7b05327.
Kitamura, M., R. Yuasa, and D. L. Van Vranken (2015), Synthesis of the cyclic prenylguanidine nitensidine E using a palladium-catalyzed carbenylative amination, *Tetrahedron Letters*, *56*(23), 3027-3031, doi:10.1016/j.tetlet.2014.10.140.
Kohn, B. L., N. Ichiishi, and E. R. Jarvo (2013), Silver-Catalyzed Allenylation and Enantioselective Propargylation Reactions of Ketones, *Angewandte Chemie-International Edition*, *52*(16), 4414-4417, doi:10.1002/anie.201206971.
Kotyk, J. F. K., C. M. Hanna, R. L. Combs, J. W. Ziller, and J. Y. Yang (2018), Intramolecular hydrogen-bonding in a cobalt aqua complex and electrochemical water oxidation activity, *Chem. Sci.*, *9*(10), 2750-2755, doi:10.1039/c7sc04960a.
Kreutzer, A. G., I. L. Harnza, R. K. Spencer, and J. S. Nowick (2016), X-ray Crystallographic Structures of a Trimer, Dodecamer, and Annular Pore Formed by an Ab(17)_(36) beta-Hairpin, *J. Amer. Chem. Soc.*, *138*(13), 4634-4642, doi:10.1021/jacs.6b01332.
Kreutzer, A. G., R. K. Spencer, K. J. McKnelly, S. Yoo, I. L. Hamza, P. J. Salveson, and J. S. Nowick (2017), A Hexamer of a Peptide Derived from Aβ(16-36), *Biochemistry*, *56*(45), 6061-6071, doi:10.1021/acs.biochem.7b00831.
Kyrychenko, A., N. M. Lim, V. Vasquez-Montes, M. V. Rodnin, J. A. Freites, L. P. Nguyen, D. J. Tobias, D. L. Mobley, and A. S. Ladokhin (2018), Refining Protein Penetration into the Lipid Bilayer Using Fluorescence Quenching and Molecular Dynamics Simulations: The Case of Diphtheria Toxin Translocation Domain, *Journal of Membrane Biology*, *251*(3), 379-391, doi:10.1007/s00232-018-0030-2.
Langeslay, R. R., G. P. Chen, C. J. Windorff, A. K. Chan, J. W. Ziller, F. Furche, and W. J. Evans (2017), Synthesis, Structure, and Reactivity of the Sterically Crowded Th3+ Complex (C5Me5)(3)Th Including Formation of the Thorium Carbonyl, (C5Me5)(3)Th(CO) BPh4, *J. Amer. Chem. Soc.*, *139*(9), 3387-3398, doi:10.1021/jacs.6b10826.
Li, L., J. C. Snyder, I. M. Pelaschier, J. Huang, U. N. Niranjan, P. Duncan, M. Rupp, K. R. Muller, and K. Burke (2016), Understanding machine-learned density functionals, *International Journal of Quantum Chemistry*, *116*(11), 819-833, doi:10.1002/qua.25040.
Lignell, H., S. A. Epstein, M. R. Marvin, D. Shemesh, R. B. Gerber, and S. Nizkorodov (2013), Experimental and Theoretical Study of Aqueous cis-Pinonic Acid Photolysis, *J. Phys. Chem. A*, *117*(48), 12930-12945, doi:10.1021/jp4093018.
Liu, M. D., et al. (2018), Statistical Coupling Analysis-guided library design for discovery of mutant luciferases, *Biochemistry*, *in press*.
Liu, S., S. Cao, K. Hoang, K. L. Young, A. S. Paluch, and D. L. Mobley (2016), Using MD Simulations To Calculate How Solvents Modulate Solubility, *Journal of Chemical Theory and Computation*, *12*(4), 1930-1941, doi:10.1021/acs.jctc.5b00934.
Liu, Y., M. Gibbs, C. L. Perkins, J. Tolentino, M. H. Zarghami, J. Bustamante, and M. Law (2011), Robust, Functional Nanocrystal Solids by Infilling with Atomic Layer Deposition, *Nano Letters*, *11*(12), 5349-5355, doi:10.1021/nl2028848.
Lydon, B. R., A. Germann, and J. Y. Yang (2016), Chemical modification of gold electrodes via non-covalent interactions, *Inorganic Chemistry Frontiers*, *3*(6), 836-841, doi:10.1039/c6qi00010j.
MacMillan, A. C., J. B. Morrison, C. W. Harmon, and S. A. Nizkorodov (2012), Enhancement of Surfactants in Nanoparticles Produced by an Electrospray Aerosol Generator, *Aerosol Sci. Technol.*, *46*(11), 1239-1245, doi:10.1080/02786826.2012.708946.

Malecha, K. T., Z. C. Cai, and S. A. Nizkorodov (2018), Photodegradation of Secondary Organic Aerosol Material Quantified with a Quartz Crystal Microbalance, *Environ. Sci. Technol. Lett.*, *5*(6), 366-371, doi:10.1021/acs.estlett.8b00231.
Mang, S. A., M. L. Walser, S. A. Nizkorodov, and J. M. Laux (2009), Measurement of Ozone Emission and Particle Removal Rates from Portable Air Purifiers, *Journal of Chemical Education*, *86*(2), 219-221, doi:10.1021/ed086p219.
Mehra, A., et al. (2020), Oligomer and highly oxygenated organic molecule formation from oxidation of oxygenated monoterpenes emitted by California sage plants, *Atmos. Chem. Phys.*, *20*(18), 10953-10965, doi:10.5194/acp-20-10953-2020.
Miller, S. M., R. A. Samame, and S. D. Rychnovsky (2012), Nanomole-Scale Assignment of Configuration for Primary Amines Using a Kinetic Resolution Strategy, *J. Amer. Chem. Soc.*, *134*(50), 20318-20321, doi:10.1021/ja310620c.
Mobley, D. L., S. Liu, N. M. Lim, K. L. Wymer, A. L. Perryman, S. Forli, N. J. Deng, J. Su, K. Branson, and A. J. Olson (2014), Blind prediction of HIV integrase binding from the SAMPL4 challenge, *Journal of Computer-Aided Molecular Design*, *28*(4), 327-345, doi:10.1007/s10822-014-9723-5.
Nguyen, C. Q., et al. (2018), Longitudinal Monitoring of Biofilm Formation via Robust Surface-Enhanced Raman Scattering Quantification of Pseudomonas aeruginosa-Produced Metabolites, *ACS Applied Materials & Interfaces*, *10*(15), 12364-12373, doi:10.1021/acsami.7b18592.
Nguyen, T. B., P. B. Lee, K. M. Updyke, D. L. Bones, J. Laskin, A. Laskin, and S. A. Nizkorodov (2012), Formation of nitrogen- and sulfur-containing light-absorbing compounds accelerated by evaporation of water from secondary organic aerosols, *J. Geophys. Res. D*, *117*, D01207, doi:01210.01029/02011JD016944, doi:10.1029/2011jd016944.
Ogata, A. F., J. M. Edgar, S. Majumdar, J. S. Briggs, S. V. Patterson, M. X. Tan, S. T. Kudlacek, C. A. Schneider, G. A. Weiss, and R. M. Penner (2017), Virus-Enabled Biosensor for Human Serum Albumin, *Anal. Chem.*, *89*(2), 1373-1381, doi:10.1021/acs.analchem.6b04840.
Palumbo, C. T., et al. (2018), Metal versus Ligand Reduction in Ln(3+) Complexes of a Mesitylene-Anchored Tris(Aryloxide) Ligand, *Inorganic Chemistry*, *57*(5), 2823-2833, doi:10.1021/acs.inorgchem.7b03236.
Passalacqua, L. F. M., A. I. Dingilian, and A. Luptak (2020), Single-pass transcription by T7 RNA polymerase, *Rna*, *26*(12), 2062-2071, doi:10.1261/rna.076778.120.
Passalacqua, L. F. M., R. M. Jimenez, J. Y. Fong, and A. Luptak (2017), Allosteric Modulation of the Faecalibacterium prausnitzii Hepatitis Delta Virus-like Ribozyme by Glucosamine 6-Phosphate: The Substrate of the Adjacent Gene Product, *Biochemistry*, *56*(45), 6006-6014, doi:10.1021/acs.biochem.7b00879.
Pevarnik, M., K. Healy, M. Davenport, J. Yen, and Z. S. Siwy (2012), A hydrophobic entrance enhances ion current rectification and induces dewetting in asymmetric nanopores, *Analyst*, *137*(13), 2944-2950, doi:10.1039/c2an16139g.
Powell, M. R., M. Sullivan, I. Vlassiouk, D. Constantin, O. Sudre, C. C. Martens, R. S. Eisenberg, and Z. S. Siwy (2008), Nanoprecipitation-assisted ion current oscillations, *Nature Nanotechnology*, *3*(1), 51-57, doi:10.1038/nnano.2007.420.
Premachandra, I., T. A. Nguyen, C. T. Shen, E. S. Gutman, and D. L. Van Vranken (2015), Carbenylative Amination and Alkylation of Vinyl Iodides via Palladium Alkylidene Intermediates, *Organic Letters*, *17*(21), 5464-5467, doi:10.1021/acs.orglett.5b02820.
Qiu, Y. H., et al. (2015), Pores with Longitudinal Irregularities Distinguish Objects by Shape, *Acs Nano*, *9*(4), 4390-4397, doi:10.1021/acsnano.5b00877.
Rathbun, C. M., W. B. Porterfield, K. A. Jones, M. J. Sagoe, M. R. Reyes, C. T. Hua, and J. A. Prescher (2017), Parallel Screening for Rapid Identification of Orthogonal Bioluminescent Tools, *ACS Cent. Sci.*, *3*(12), 1254-1261, doi:10.1021/acscentsci.7b00394.
Romonosky, D. E., N. N. Ali, M. N. Saiduddin, M. Wu, H. J. Lee, P. K. Aiona, and S. A. Nizkorodov (2016), Effective absorption cross sections and photolysis rates of anthropogenic

and biogenic secondary organic aerosols, *Atmos. Environ.*, *130*, 172-179, doi:10.1016/j.atmosenv.2015.10.019.
Romonosky, D. E., L. Q. Nguyen, D. Shemesh, T. B. Nguyen, S. A. Epstein, D. B. C. Martin, C. D. Vanderwal, R. B. Gerber, and S. A. Nizkorodov (2015), Absorption spectra and aqueous photochemistry of beta-hydroxyalkyl nitrates of atmospheric interest, *Molecular Physics*, *113*(15-16), 2179-2190, doi:10.1080/00268976.2015.1017020.
Salveson, P. J., S. Haerianardakani, A. G. Kreutzer, and J. S. Nowick (2018), Controlling the Oligomerization State of Aβ-Derived Peptides with Light, *J. Amer. Chem. Soc.*, *140*(17), 5842-5852, doi:10.1021/jacs.8b02658.
Samame, R. A., C. M. Owens, and S. D. Rychnovsky (2016), Concise synthesis of (+)-fastigiatine, *Chem. Sci.*, *7*(1), 188-190, doi:10.1039/c5sc03262h.
Schow, E. V., J. A. Freites, A. Nizkorodov, S. H. White, and D. J. Tobias (2012), Coupling between the voltage-sensing and pore domains in a voltage-gated potassium channel, *Biochimica Et Biophysica Acta-Biomembranes*, *1818*(7), 1726-1736, doi:10.1016/j.bbamem.2012.02.029.
Shaffer, D. W., I. Bhowmick, A. L. Rheingold, C. Tsay, B. N. Livesay, M. P. Shores, and J. Y. Yang (2016), Spin-state diversity in a series of Co(II) PNP pincer bromide complexes, *Dalton Transactions*, *45*(44), 17910-17917, doi:10.1039/c6dt03461f.
Steinhardt, R. C., J. M. O'Neill, C. M. Rathbun, D. C. McCutcheon, M. A. Paley, and J. A. Prescher (2016), Design and Synthesis of an Alkynyl Luciferin Analogue for Bioluminescence Imaging, *Chemistry – A European Journal*, *22*(11), 3671-3675, doi:10.1002/chem.201503944.
Steinhardt, R. C., et al. (2017), Brominated Luciferins Are Versatile Bioluminescent Probes, *Chembiochem*, *18*(1), 96-100, doi:10.1002/cbic.201600564.
Sutthirat, N., Z. Zhammavongsy, D. W. Cunningham, R. J. Eisenhart, J. W. Ziller, and J. Y. Yang (2018), Adaptable Ligand Donor Strength: Tracking Transannular Bond Interactions in Tris(2-pyridylmethyl)-azaphosphatrane, *Dalton Transactions*, *47*, 14101-14110.
Sutthirat, N., J. W. Ziller, J. Y. Yang, and Z. Thammavongsy (2019), Crystal structure of NiFe(CO)5[tris(pyridylmethyl)azaphosphatrane]: a synthetic mimic of the NiFe hydrogenase active site incorporating a pendant pyridine base, *Acta Crystallographica Section E*, *75*(4), 438-442, doi:10.1107/S2056989019003256.
Tadayon, S. V., E. S. Foreman, and C. Murray (2018), Kinetics of the Reactions between the Criegee Intermediate CH2OO and Alcohols, *J. Phys. Chem. A*, *122*(1), 258-268, doi:10.1021/acs.jpca.7b09773.
Tao, D. J., Y. Slutskyy, M. Muuronen, A. Le, P. Kohler, and L. E. Overman (2018), Total Synthesis of (−)-Chromodorolide B By a Computationally-Guided Radical Addition/Cyclization/Fragmentation Cascade, *J. Amer. Chem. Soc.*, *140*(8), 3091-3102, doi:10.1021/jacs.7b13799.
Tay, G. C., C. Y. Huang, and S. D. Rychnovsky (2014), Silyl Enol Ether Prins Cyclization: Diastereoselective Formation of Substituted Tetrahydropyran-4-ones, *Journal of Organic Chemistry*, *79*(18), 8733-8749, doi:10.1021/jo501580p.
Thammavongsy, Z., I. M. Kha, J. W. Ziller, and J. Y. Yang (2016), Electronic and steric Tolman parameters for proazaphosphatranes, the superbase core of the tri(pyridylmethyl)azaphosphatrane (TPAP) ligand, *Dalton Transactions*, *45*(24), 9853-9859, doi:10.1039/c6dt00326e.
Thrift, W. J., et al. (2017), Driving Chemical Reactions in Plasmonic Nanogaps with Electrohydrodynamic Flow, *ACS Nano*, *11*(11), 11317-11329, doi:10.1021/acsnano.7b05815.
Tkacz, K., S. T. E. Nitz, W. White, and S. Ardo (2017), Investigating Saltwater Desalination by Electrodialysis and Curriculum Extensions To Introduce Students to the Chemical Physics of Polymeric Ion-Exchange Membranes, *Journal of Chemical Education*, *94*(11), 1733-1737.
Tran, A., G. Williams, S. Younus, N. N. Ali, S. L. Blair, S. A. Nizkorodov, and H. A. Al-Abadleh (2017), Efficient Formation of Light-Absorbing Polymeric Nanoparticles from the Reaction of

Soluble Fe(III) with C4 and C6 Dicarboxylic Acids, *Environ. Sci. Technol.*, *51*(17), 9700-9708, doi:10.1021/acs.est.7b01826.
Tsay, C., B. N. Livesay, S. Ruelas, and J. Y. Yang (2015), Solvation Effects on Transition Metal Hydricity, *J. Amer. Chem. Soc.*, *137*(44), 14114-14121, doi:10.1021/jacs.5b07777.
Unhelkar, M. H., V. T. Duong, K. N. Enendu, J. E. Kelly, S. Tahir, C. T. Butts, and R. W. Martin (2017), Structure prediction and network analysis of chitinases from the Cape sundew, Drosera capensis, *Biochimica Et Biophysica Acta-General Subjects*, *1861*(3), 636-643, doi:10.1016/j.bbagen.2016.12.007.
Updyke, K. M., T. B. Nguyen, and S. A. Nizkorodov (2012), Formation of brown carbon via reactions of ammonia with secondary organic aerosols from biogenic and anthropogenic precursors, *Atmos. Environ.*, *63*, 22-31, doi:10.1016/j.atmosenv.2012.09.012.
Vander Wall, A. C., V. Perraud, L. M. Wingen, and B. J. Finlayson-Pitts (2020), Evidence for a kinetically controlled burying mechanism for growth of high viscosity secondary organic aerosol, *Environ. Sci.: Processes Impacts*, *22*(1), 66-83, doi:10.1039/c9em00379g.
Vincent, J. C., M. Muuronen, K. C. Pearce, L. N. Mohanam, E. Tapavicza, and F. Furche (2016), That Little Extra Kick: Nonadiabatic Effects in Acetaldehyde Photodissociation, *Journal of Physical Chemistry Letters*, *7*(20), 4185-4190, doi:10.1021/acs.jpclett.6b02037.
Vu, K., J. C. Snyder, L. Li, M. Rupp, B. F. Chen, T. Khelif, K. R. Mueller, and K. Burke (2015), Understanding kernel ridge regression: Common behaviors from simple functions to density functionals, *International Journal of Quantum Chemistry*, *115*(16), 1115-1128, doi:10.1002/qua.24939.
Vu, M. M. K., N. E. Jameson, S. J. Masuda, D. Lin, R. Larraide-Ridaura, and A. Luptak (2012), Convergent Evolution of Adenosine Aptamers Spanning Bacterial, Human, and Random Sequences Revealed by Structure-Based Bioinformatics and Genomic SELEX, *Chemistry & Biology*, *19*(10), 1247-1254, doi:10.1016/j.chembiol.2012.08.010.
Wagner, A. J., J. G. David, and S. D. Rychnovsky (2011), Determination of Absolute Configuration Using Kinetic Resolution Catalysts, *Organic Letters*, *13*(16), 4470-4473, doi:10.1021/ol201902y.
Wagner, A. J., S. M. Miller, R. P. King, and S. D. Rychnovsky (2016), Nanomole-Scale Assignment and One-Use Kits for Determining the Absolute Configuration of Secondary Alcohols, *Journal of Organic Chemistry*, *81*(15), 6253-6265, doi:10.1021/acs.joc.6b00816.
Wagner, A. J., S. M. Miller, S. Nguyen, G. Y. Lee, S. D. Rychnovsky, and R. D. Link (2014), Undergraduate Laboratory Experiment To Determine Absolute Configuration Using Thin-Layer Chromatography, *Journal of Chemical Education*, *91*(5), 716-721, doi:10.1021/ed4004996.
Wang, Y. L., N. L. Truex, N. D. P. Vo, and J. S. Nowick (2018), Effects of charge and hydrophobicity on the oligomerization of peptides derived from IAPP, *Bioorg. Med. Chem.*, *26*(6), 1151-1156, doi:10.1016/j.bmc.2017.10.001.
Wingen, L. M., and B. J. Finlayson-Pitts (2019), Probing surfaces of atmospherically relevant organic particles by easy ambient sonic-spray ionization mass spectrometry (EASI-MS), *Chem. Sci.*, *10*(3), 884-897, doi:10.1039/c8sc03851a.
Yang, H., D. R. Du Bois, J. W. Ziller, and J. S. Nowick (2017), X-ray crystallographic structure of a teixobactin analogue reveals key interactions of the teixobactin pharmacophore, *Chemical Communications*, *53*(18), 2772-2775, doi:10.1039/c7cc00783c.
Yuan, T. Z., et al. (2015), Shear-Stress-Mediated Refolding of Proteins from Aggregates and Inclusion Bodies, *Chembiochem*, *16*(3), 393-396, doi:10.1002/cbic.201402427.
Zarghami, M. H., Y. Liu, M. Gibbs, E. Gebremichael, C. Webster, and M. Law (2010), p-Type PbSe and PbS Quantum Dot Solids Prepared with Short-Chain Acids and Diacids, *Acs Nano*, *4*(4), 2475-2485, doi:10.1021/nn100339b.