UNIVERSITY OF THE
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Dr. Anthony Dutoi
Department of Chemistry

Faculty profile link
Research lab link
Email: adutoi@pacific.edu

PROJECT TITLE

Analysis of Femtosecond Time-resolved X-ray Transient Absorption Spectra (1 student)

MINIMUM REQUIRED SKILLS

- Experience with Linux and Python.
- Working knowledge of the time-dependent Schrödinger equation and Fourier transforms.
- Good working ethics, team work spirit, and English communication skill.

SCHOLARLY SIGNIFICANCE

The high-harmonic generation process produces soft X-ray pulses that have the potential to be shorter than a single femtosecond, offering unprecedented time resolution in the study of coherent quantum molecular dynamics. Furthermore, though technically advanced, these devices are of table-top dimension, meaning they may someday form the basis of widespread investigative techniques. However, as with most modern time-resolved spectroscopic methods, experimental spectra are very difficult to interpret without the aid of theory. This project aims to demonstrate and advance the extent to which experimental methods may be used to directly reconstruct the time-dependent wavefunctions produced in the laboratory in simple (diatomic) molecules.

PROJECT OBJECTIVES

1. Analyze the complex phase information associated with the frequency components of a simulated time-domain experiment.
2. Demonstrate the procedure by which a quantum vibrational wavepacket may be recovered from the Fourier transform of a time-domain X-ray absorption signal.

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will learn how to interpret cutting-edge experiments that employ X-ray absorption for fine time-resolution of molecular dynamics. They will have the opportunity to develop applied programming skills.

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Dr. Andreas H. Franz
Department of Chemistry

Faculty profile link
Research lab link
Email: afranz@pacific.edu

PROJECT TITLE

Conformational analysis of oligosaccharides (1-2 students)

MINIMUM REQUIRED SKILLS

- Previous lab experience is highly preferred.
- Knowledge in analytical and organic chemistry is preferred.
- Good working ethics, team work spirit, and English communication skill are required.

SCHOLARLY SIGNIFICANCE

Oligosaccharides play a multitude of roles in biochemical processes. Their potential structural diversity is stunning; however, for unknown reasons, nature appears to use only a comparatively small number of sugar structures in its biochemical machinery. Not only do glycans contain a "sugar code" as far as constitution, configuration, anomericity, and chemical modifications are concerned, but also in terms of time-averaged solution conformation. Dr. Franz's group combines organic chemistry, magnetic resonance spectroscopy (NMR), and molecular modeling to study the conformational flexibility of oligosaccharides.

PROJECT OBJECTIVES

1. NMR analysis of commercial and synthetic glycans
2. Coupling constant analysis
3. Molecular dynamics simulation and comparison to NMR data

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will conduct magnetic resonance experiments, collect/interpret data, and learn how to setup/run/analyze molecular dynamics simulations. Simple synthetic laboratory skills may be included such as reaction monitoring, distillation, and column chromatography.

UNIVERSITY OF THE
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Dr. Joseph Harrison
Department of Chemistry

Faculty profile link

Email: jharrison@pacific.edu

PROJECT TITLE

Developing inhibitors of ubiquitin pathways (1-2 students)

MINIMUM REQUIRED SKILLS

- Enthusiasm and creativity are required!
- Knowledge of molecular biology and biochemistry is helpful, but not required.
- Experience with computational techniques is required for one project.

SCHOLARLY SIGNIFICANCE

Ubiquitin is a protein post-translational modification that controls the fate of cellular proteins. Ubiquitin is also emerging as an important signal in epigenetics. Furthermore, many diseases, such as cancer, result from alterations to the ubiquitin pathway. Likewise, ubiquitin pathways are emerging as target for drug design and there are clinically approved drugs being used that target the ubiquitin pathway. The research in my lab is focused on ubiquitin discovery. Here we use biochemical and computational methods to understand ubiquitin pathways in order to develop designed protein and small-molecule inhibitors of this pathway.

PROJECT OBJECTIVES

1. Express proteins from the ubiquitin pathway in *E. coli*
2. Perform enzymatic assays and analyze the products
3. Computational simulation and database construction/analysis of ubiquitin database

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will perform standard molecular biology experiments to clone new proteins, purify proteins from bacterial sources, and conduct enzymatic and biochemical assays on these purified proteins. The student may also use the computational design software Rosetta to model mutations and develop a database of ubiquitin interactions.

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Dr. C. Michael McCallum
Department of Chemistry

Faculty profile link
Research lab link
Email: mmccallum@pacific.edu

PROJECT TITLE

Response of hydrogen bonds in peptides to mechanical stress (1 student)

MINIMUM REQUIRED SKILLS

- Experience with UNIX/Linux or OS X computers.
- Some knowledge of programming and/or scripting highly desirable (Python/Tk/TCL/Perl or structured languages) .
- Good working ethics, team spirit, and English communication skill are required.

SCHOLARLY SIGNIFICANCE

Hydrogen bonds are known to be critical to the protein folding process, as well as the stabilization of folded protein structure. The exact process – timing, order, and strength – of hydrogen bond formation is open to analysis. The method of steered molecular dynamics (SMD) offers a way towards better understanding the role of hydrogen bonding in protein folding. Simply put, a folded peptide or protein is virtually pulled apart in a simulation. The strength of the original hydrogen bonds may be measured as they individually break, and repeated simulations may give information about preference or ordering. This may allow steering the simulation in the forward (folding) direction in order to find a correct folding pathway.

PROJECT OBJECTIVES

1. Setup and simulation equilibrium protein simulations
2. Determine effective pulling methods and modes useful to analyze hydrogen bonds
3. Analyze data obtained and inform further SMD experiments

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will utilize modern simulation packages (CHARMM/NAMD/Gromacs/Amber) to perform SMD computer simulations and analyze the results. The student will learn useful scripting and programming skills in addition to the MD techniques.

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Dr. Jianhua Ren
Department of Chemistry

Faculty profile link
Research lab link
Email: jren@pacific.edu

PROJECT TITLE

Synthesis and characterization of peptides and peptoids (1-2 students)

MINIMUM REQUIRED SKILLS

- Knowledge in analytical chemistry, organic chemistry and physical chemistry
- Previous lab experience is highly favorable
- Be able to communicate in English and to work independently

SCHOLARLY SIGNIFICANCE

Peptides are natural biopolymers. Peptides can be used as a model to study the influence of conformational changes on the chemical properties in biopolymers. Peptoids are peptide-mimicking polymers that are able to fold into peptide-like secondary structures, and even into protein-like tertiary architectures. Dr. Ren's lab focuses on utilizing tandem mass spectrometry techniques and computational methods to study the structural features and chemical properties of peptides and peptoids, and their applications in biological systems.

PROJECT OBJECTIVES

1. Synthesis of peptides and peptoids
2. Sequencing peptides and peptoids by using mass spectrometry techniques
3. Molecular modeling

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The students will learn and carry out peptide and peptoid synthesis using a method developed in Dr. Ren's lab. The students will work with graduate students closely to perform mass spectrometry measurements using an LCMS spectrometer, and to characterize the fragmentation patterns of peptides and peptoids. The students will learn how to use Spartan and Gaussian computational software to calculate the structures of peptides and peptoids.

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Dr. Balint Sztaray
Department of Chemistry

Faculty profile link
Research lab link
Email: bsztaray@pacific.edu

PROJECT TITLE

Isomer-Resolved Detection of Cyano Radical Reaction Products for Predictive Chemical Models of Extra-Terrestrial Atmospheres (1-2 students)

MINIMUM REQUIRED SKILLS

- Good computer and calculation skills are necessary.
- Knowledge in physical chemistry (thermochemistry, kinetics) is preferred.
- Good working ethics and good English communication skills are required.

SCHOLARLY SIGNIFICANCE

The atmosphere of extra-terrestrial objects has been extensively examined using theoretical and experimental Earth-based studies, and space missions, as well. The particular interest in Titan, the largest moon of Saturn, lies in its atmospheric composition, which might be similar to that of the Earth's early atmosphere. Molecular nitrogen, methane, hydrogen, and nitrogen-containing small molecules are the most abundant species found in Titan's atmosphere. In this environment, the main source of the CN radical is the photolysis of hydrogen cyanide. Therefore, its reaction with unsaturated hydrocarbons is of great interest in the development of reliable photochemical models of this astrochemical environment.

PROJECT OBJECTIVES

1. Analysis of Photoelectron Photoion Coincidence (PEPICO) spectroscopy data that we collected on CN + hydrocarbon reactions.
2. Quantum-chemical calculations on the reaction involved.

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will use proprietary software to analyze the raw PEPICO data files that will have been collected at the Swiss Light Source synchrotron. Reaction products will be identified and quantified based on their mass and their photoelectron spectra. Reaction pathways will be investigated using ab initio and DFT quantum-chemical methods.

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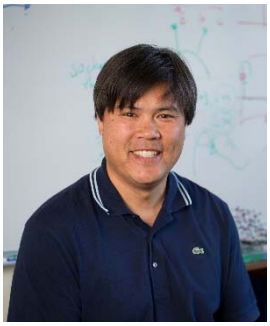

Dr. Jerry Tsai
Department of Chemistry

Faculty profile link
Research lab link
Email: jtsai@pacific.edu

PROJECT TITLE

Defining the Amino Acid Code to Protein Packing (1-2 students)

MINIMUM REQUIRED SKILLS

- 1 year of General Chemistry, Organic Chemistry, Biology, Math, & Physics
- Positive attitude and ability to work independently/problem solve on their own
- Basic proficiency in written and spoken English

SCHOLARLY SIGNIFICANCE

The purpose of this project is to determine the amino acid code to protein packing in tertiary and quaternary protein structure. The central concept is that a simple 4 residue knob-socket construct can simply and intuitively describe the protein packing. Both computational and experimental studies are undertaken. The computational analysis involves detailed investigation of the amino acid composition of residues packing in knob-sockets at the individual as well as in describing systems of interactions. Experimental work investigates the knob-socket predictive abilities in protein design, expression, purification, and characterization studies. The results will have significant impact on the basic understanding of how protein sequence determines protein structure.

PROJECT OBJECTIVES

1. Computational analysis of protein knob-socket packing structure
2. Experimental protein design using the knob-socket motif

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

Overall, students will learn about the fundamentals of protein structure. Specifically in the computational studies, students will learn the basics of programming and data mining. In the experimental studies, students will learn techniques in molecular biology and biochemistry.

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Dr. Vyacheslav Samoshin
Department of Chemistry

Faculty profile link
Research lab link
Email: vsamoshin@pacific.edu

PROJECT TITLE

Synthesis and studies of novel conformational switches (1-2 students)

MINIMUM REQUIRED SKILLS

- Knowledge in organic chemistry (1 year) and undergraduate lab experience are required.
- Previous research lab experience is highly favorable.
- Good working ethics and basic proficiency in written and spoken English are required.

SCHOLARLY SIGNIFICANCE

The development of molecular switches (triggers) is of great current interest in view of their possible use in many applications, such as drug release, new sensor techniques or information storage and transmission. Molecular switches are molecules that can reversibly change their properties under external influence. New compounds of this type, which can switch their conformation, are currently synthesized and studied in Dr. Samoshin's group, especially as the controllable lipid-like components of the acid-triggerable liposomes for targeted drug and gene delivery.

PROJECT OBJECTIVES

1. Synthesis of new molecular switches.
2. Studies of their conformational changes in various conditions by NMR spectroscopy.
3. Exploration of these compounds as the triggerable liposome components.

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will conduct multistep organic synthesis using basic techniques and characterize the structure and conformational properties of products using NMR spectroscopy and mass spectrometry. The student will also participate in preparation and studies of acid-triggerable liposomes.

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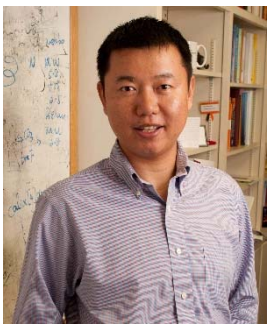

Dr. Liang Xue
Department of Chemistry

Faculty profile link
Research lab link
Email: lxue@pacific.edu

PROJECT TITLE

Decomposition of organic molecules by photosensitizers (1-2 students)

MINIMUM REQUIRED SKILLS

- Previous lab experience is highly favorable.
- Knowledge in analytical and organic chemistry is preferred.
- Good working ethics, team work spirit, and English communication skill are required.

SCHOLARLY SIGNIFICANCE

Flavin based catalysts have been developed to promote redox reactions in many applications such as bioremediation and wastewater treatment in recent years. Examples include the reduction of carbon-carbon double bonds using organocatalytically generated diimide by 5-ethyl riboflavin, reduction of olefins by synthetic flavin catalysts *In Situ, and* flavin-sensitized photooxidaton of substituted phenols in natural water. Dr. Xue's group combines organic chemistry and mass spectrometry to study the decomposition of phenol derivatives that are environmental toxins from industry.

PROJECT OBJECTIVES

1. Synthesis of flavin derivatives
2. Decomposition of phenols by flavin derivatives under sunlight
3. Analysis of reaction products using high-resolution GC mass spectrometry

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will conduct multistep organic synthesis using basic techniques including distillation and column chromatography. The student will also use high resolution GC mass spectrometry to establish calibration curves and determine reaction products.

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Dr. Qinliang Zhao
Department of Chemistry

Faculty profile link
Research lab link
Email: lxue@pacific.edu

PROJECT TITLE

Design and synthesis of complexes for catalyst development (1-2 students)

MINIMUM REQUIRED SKILLS

- Experience in organic and inorganic synthesis and characterization
- Knowledge in organic and coordination chemistry.
- Good working ethics, team work spirit, and English communication skill.

SCHOLARLY SIGNIFICANCE

Developing metal complexes of interesting properties toward catalysis has been an important research area especially since the dramatic increase in need for industry and pharmacy. Our group focuses on utilizing ligand function and coordination chemistry to assemble new complexes and then study their reactivities. Tuning both the ligand framework and the metal center could adjust the complexes' properties that could lead to the desired reactivities.

PROJECT OBJECTIVES

1. Synthesis of polydentate ligands
2. Assembling and characterization of metal-containing complexes
3. Exploring reactivities with various reagents

METHODS/TECHNIQUES/INSTRUMENTS TO BE LEARNED/USED

The student will conduct multistep organic and inorganic synthesis using basic techniques including Schlenk line operation, precipitation, crystallization, and column chromatography. The student will use NMR, MS, HPLC, Echem and X-ray diffraction to characterize the product.