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**Please refer to www.nyu.edu/pages/chemistry to learn more about Professors Canary & Tuckerman.

Chemistry Undergraduate Research @ NYU

http://www.nyu.edu/clubs/drapersociety

Prospective Researchers:

We are encouraged by your interest in chemistry research here at New York University. This letter is designed as a guide to the event and beginning research at NYU.

In this guide you will find descriptions for various opportunities available in the chemistry department for undergraduate research. Please note that this guide is by no means all-inclusive. Remember there are other interesting opportunities available in the chemistry department itself, in other NYU departments, at the medical school, and at outside research institutes. While this may seem very overwhelming, we hope that this guide is a good starting point for your quest for the right research group.

The type of research is split up into two main categories: Experimental & Theoretical. Experimental chemistry includes the wet-chemistry that you have experienced in general chemistry and organic chemistry labs. Moreover, it also includes such things as spectroscopy (i.e. Nuclear Magnetic Resonance or Mass Spectroscopy). Generally, this work requires the handling of actual chemicals. Theoretical work, on the other hand, does not involve these types of experiments. Theoretical work is largely dependent on computing and mathematical models of real systems. A theoreticians 'lab' is in large part a pad of paper and a computer terminal. Within these two broad headings there are further sub-categories such as organic chemistry, physical chemistry, quantum mechanics, biochemistry, etc…

When trying to find a lab that suits you, do not be discouraged if you feel you are inexperienced. Instead, try to find a lab that is interesting to you. Chances are the lab will be willing to train you if you are enthusiastic enough. So do not be discouraged if you have not had organic chemistry yet and do not know synthesis, if you have never analyzed NMR data before, or even if you do not know a programming language.

This guide is designed to introduce you to opportunities available in the department. However, at the end of the day, it is your job to contact the professors and meet with them regarding research opportunities. Even if you just want to meet with them to learn more about their work, do not hesitate to contact the professors to further investigate what really appeals to you.

Happy hunting!
Draper Chemistry Society E-board

This guide was prepared by Yael Elmatad and the Draper Society E-board with the help of many professors and researchers who worked on the descriptions you see here. December 2004.

Professor Paramjit Arora

Organic Chemistry/Biological Chemistry (Experimental)

General Overview of Research:

My lab is interested in the synthesis of organic molecules for their potential use in the control of protein-protein interactions. We make molecules that mimic structural motifs found within proteins in order to reproduce or inhibit the function of a given protein.

Responsibilities of an Undergraduate Researcher:

The NYU Chemistry Department considers the training of undergraduate students to be an integral part of a faculty member's job description. The goal of the department is to prepare undergraduate students for further studies in the Graduate School (or Medical School). I try to start undergraduate students off slowly by having them learn the basics of bioorganic chemistry under the guidance of a graduate student or a postdoctoral fellow. After the basic training has completed (which typically takes 6-12 months), the undergraduate student is treated as any other researcher in the lab is afforded the appropriate responsibilities.

Availability Requirement for Undergraduates:

My hope is to accept only those students into my lab who are genuinely interested in becoming a well-trained scientist. It is difficult to become a competent researcher in a short period of time. I have been very lucky so far that the students that have joined my group have been incredibly dedicated and hard working. They decide their own schedules but typically put in about 20 hours per week during the school year into their independent research.

Course / Previous Experience Requirements for Undergraduates:

Since our research is centered on organic chemistry, a basic set of knowledge through courses (the standard one year of organic chemistry course with lab) is a necessary prerequisite to join our lab. As mentioned above, it requires a 6-12 months of training before a student becomes a competent researcher, so I prefer to take undergraduate students who are just finishing their sophomore year and are willing to spend the next two years (including summers) in the lab.

Contact Information:

Professor Arora's Email: arora@nyu.edu

Professor Zlatko Bacic

Computational & Quantum Chemistry (Theoretical)

General Overview of Research:

Our group is concerned with structures of small molecule clusters. We examine potential energy surfaces (PESs) with many minima and try to obtain a set of structures (both global and local minima). Previously examined clusters include $(H_2)_n$, HF-$(H2)_n$, and HF-$(Ar)_n$. Current clusters of interest include CO-$(H_2)_n$ and HCl_2-$(He)_n$. We are also interested in fuel storage (H_2) in carbon nanotubes.

In order to probe these PESs we use methods such as simulated annealing which allows us to examine many minima and determine static equilibrium structures. Beyond static equilibrium structures, we also employ quantum Monte Carlo calculations to investigate dynamical features of these clusters.

Responsibilities of an Undergraduate Researcher:
Undergraduate researchers will take on projects often in conjunction with another member of our group. They will be asked to put together and implement computer programs to try an elucidate structures of small molecule clusters.

Availability Requirement for Undergraduates:
Students are expected to be available for 5-10 hours a week to do research. However, as it is theoretical research, work can be done wherever there is computer access.

Course / Previous Experience Requirements for Undergraduates:
A strong background in mathematics and physical chemistry is highly suggested for work in our group. Previous knowledge of a programming language (C or Fortran) is recommended, but not necessary. Students who do not know how to program will be asked to learn a language before beginning research.

Contact Information:
Professor Bacic's Email: zlatko.bacic@nyu.edu

Professor James Canary
Organic Chemistry (Experimental)

General Overview of Research:

Responsibilities of an Undergraduate Researcher:

Availability Requirement for Undergraduates:

Course / Previous Experience Requirements for Undergraduates:

Contact Information:

Professor Young-Tae Chang
Organic Chemistry/Biological Chemistry (Experimental)

General Overview of Research:
Chemical Genetics using Tagged Small Molecule Library (Young-Tae Chang)

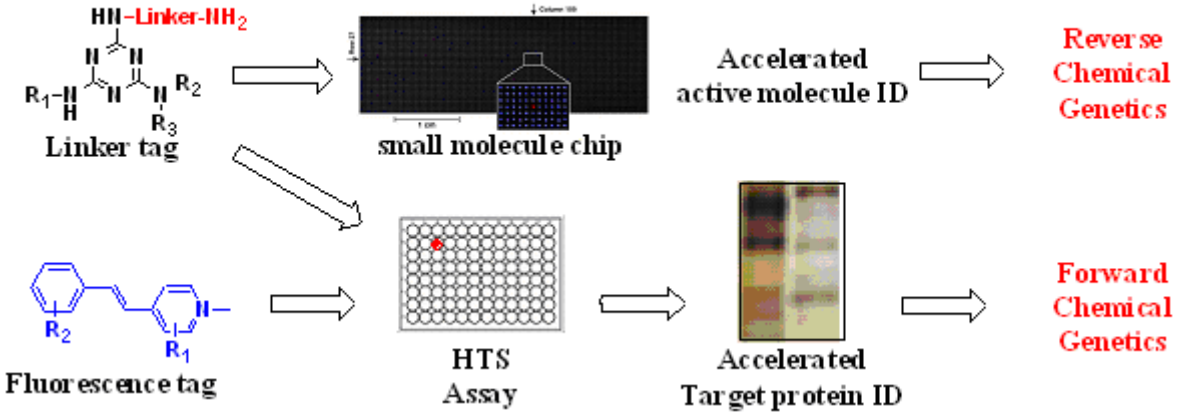
The near completion of the HGP (Human Genome Project) has conjured up a rosy dream of conquering all human disease in a short time. Unfortunately, after several years of the HGP, the real achievement or even the prospect for the advent of a "drug for everything" or the "magic drug" is not yet clear. HGP results have facilitated the identification of more drug targets (proteins) and gene functions, but it will take much

more time to connect this information to real drug development. The exponential increase of drug targets requires a new paradigm that substitutes the conventional drug development procedure. As a solution, we propose a facilitated chemical genetics using "Tagged Small Molecule Library" approach.

Elucidating the function of every gene from the sequence data of tens of thousands of genes (so called functional genomics) is the next major step for the human genome project. Geneticists have conventionally investigated the function of unknown genes by comparing the normal phenotype with that of knock-outs or through the over-expression of target genes. A novel approach utilizing chemical library screening to find an interesting phenotypic change by targeting the specific gene product, a protein, has emerged as an alternative tactic- so called ***chemical genetics***. In chemical genetics, one chemical compound may specifically inhibit or activate one (or multiple) target proteins. Therefore, the compound is equivalent to a gene knock-out or the over-expression of the gene in conventional genetics.. HGP results have facilitated the identification of more drug targets (proteins) and gene functions, but it will take much more time to connect this information to real drug development. The exponential increase of drug targets requires a new paradigm that substitutes the conventional drug development procedure. As a solution, we propose a facilitated chemical genetics using "Tagged Small Molecule Library" approach.

Although the current chemical genetics approach is very attractive, it contains intrinsically difficult steps. The biggest hurdle is the modification step of the lead compound into the affinity molecule. In order to add a linker to the lead compound without activity loss, a thorough SAR (structure-activity relationships) study is required to find the proper site of linker addition (most likely a site of the lead compound exposed to the solvent from the binding pocket of the target protein). To avoid this well-known problem, our approach is employing library molecules carrying a Tag (TL: Tagged Library) from the beginning.

Figure 2. Reverse and Forward Chemical Genetics using a Tagged Library



For further information, consult with the website at http://homepages.nyu.edu/~ytc1/

Responsibilities of an Undergraduate Researcher:

Undergraduate students in my lab start out by working alongside with a graduate student. After the training period, they will be given an independent project; at this

point they will be expected to produce significant progress, which should result in publication of the results.

Availability Requirement for Undergraduates:
It is expected that undergraduate students work 30+hours/week

Course/Previous Experience Requirements for Undergraduates:
No prior experience is required; the nature of the project will be selected accordingly.

Contact Information:
Professor Chang's Email: yt.chang@nyu.edu
Professor Chang's Phone Number: (212) 998-8491

Professor Nicholas Geacintov

Biophysical Chemistry (Experimental)

General Overview of Research:
Many chemicals, both environmental and those present in humans, damage genomic DNA. If not repaired by specialized enzymes, this damage can give rise to mutations and cancer if the DNA is incorrectly replicated or transcribed. Our laboratory is interested in the relationships between the physical, chemical, and structural characteristics of the damaged DNA, and the mechanisms of DNA repair and replication pathways. Our work is on the borderline of chemistry and molecular biology since we use most of the major tools available to chemists to study the characteristics of damaged DNA, and evaluate its fate and consequences in cellular environments (the latter experiments are performed by biologists-collaborators).

Responsibilities of an Undergraduate Researcher:
Undergraduate research usually involves working with an advanced laboratory team member, and sometimes individually, whenever feasible.

Availability Requirement for Undergraduates:
At least 12 – 15 hours/week for a meaningful experience.

Course/Previous Experience Requirements for Undergraduates:
Any lab experience is useful. Advanced High School Chemistry classes and motivation are also very important.

Contact Information:
Professor Geacintov's Email: ng1@nyu.edu

Professor Neville Kallenbach

Biological Chemistry

General Overview of Research:
Dr. Kallenbach's lab studies the physical and chemical properties of peptide folding. What are the forces that direct a peptide into it correct secondary structure given a

specific amino acid sequence. Are peptides that do not fold into either alpha helix or beta sheet random coils or do they also have a specific structure determined by the specific amino acids and their interaction with the solvent they are placed into? We are also interested in how specific peptide sequences interact with the plasma membrane of bacteria. Is the sequence, secondary and tertiary structure of these cationic antimicrobial peptides important to the interaction with the bacteria plasma membrane?

Contact Information:
Professor Kallenbach's Email: neville.kallenbach@nyu.edu

Professor Kent Kirshenbaum

Bioorganic Chemistry & Macromolecule Design (Experimental)

General Overview of Research:
We are investigating the chemical synthesis of biomimetic sequence-specific heteropolymers, and the biosynthesis of proteins incorporating unusual amino acids. Our goals are to find new avenues for the study of self-organization in macromolecules and to create innovative research tools for structural biology, biophysics, proteomics and materials science.

A major focus of our current work is in the design of agents for molecular imaging, in which we collaborate extensively with clinicians at NYU's Medical School.

Responsibilities of an Undergraduate Researcher:
A typical project for an undergrad would involve the synthesis of an unusual amino acid or monomer as a reagent for generating a macromolecule. Two of my undergraduates presented posters at the National meeting of the American Chemical Society in Philadelphia this past summer.

Availability Requirement for Undergraduates:
To accomplish anything, students typically need to spend 5 to 10 hours per week in the lab.

Course / Previous Experience Requirements for Undergraduates:
Completion (and enjoyment) of organic chemistry.

Contact Information:
Professor Kirshenbaum's Email: kent@nyu.edu
Office: Waverly Room 866

Professor Hans Schelvis

Biophysical Chemistry (Experimental)

General Overview of Research:
In our lab, we are investigating how enzymes work at the molecular level. Currently, our research efforts are concentrated on two enzymes: the DNA repair enzyme DNA photolyase, and the catalase-peroxidase from *Mycobacterium tuberculosis*, which plays

an import role in antibiotic activation. For the DNA repair enzyme, we are interested in its interactions with damaged DNA, the damage recognition process, and the actual repair process. We are also using this enzyme as a model system to study electron-transfer processes. For the tuberculosis enzyme, we are interested in the reaction mechanism that leads to antibiotic activation, and in how specific mutations affect this reaction mechanism and the enzyme structure resulting in resistance to key antibiotics. The research has a strong interdisciplinary flavor with contributions from chemistry, physics, and biology. The main research tool is resonance Raman spectroscopy, which is a technique that measures molecular vibrations. The vibrations of a molecule give a fingerprint of that molecule, which provides important information on structural changes, interactions between the molecule and it environment, and catalytic reaction intermediates. Other techniques commonly used in our lab are absorption and fluorescence spectroscopy, and HPLC purification.

Responsibilities of an Undergraduate Researcher:
We have projects for undergraduate students at all levels, but we prefer them to start in their sophomore or junior year. However, most of the undergraduate students who have worked in our lab, have started at the end of their freshman year. Many of our projects fall in the area of biophysical chemistry, and students with an interest in (bio)physical chemistry will find themselves really at home. Although some biochemistry knowledge will be helpful, there is more emphasis on the physical chemistry part. Usually, a student will first be trained in preparing buffer solutions and in collecting absorption spectra of the enzymes. Most of the projects are related to the DNA repair enzyme, and students will be trained in damaging DNA, its purification by HPLC, and the repair assay of the damaged DNA by the repair enzyme. At that point, the research can take many directions with projects that focus on the formation of DNA damage, and the effect of DNA sequence on repair, interactions with the enzyme, and electron-transfer in the enzyme. Besides research responsibilities, undergraduate students are also expected to contribute to some of the lab chores. When possible, the students are encouraged to join group meetings and to present their research at the Undergraduate Research Conference at NYU and at other meetings.

Availability Requirement for Undergraduates:
The time necessary for research in our lab depends on the project. It is best to have at least one block of 4 or more hours available during one morning or one afternoon. This time is needed to perform a significant set of experiments and/or data analysis. Availability for shorter time periods (0.5 to 1 hour) on other days for preparation of solutions is also required.

Course/Previous Experience Requirements for Undergraduates:
We are mainly looking for chemistry and biochemistry majors. Biochemistry and physical chemistry will be good courses for a student in our lab. Unfortunately, these courses are usually taken in the junior or senior year. Since we like students to start in their sophomore or junior year, we do not require these courses. We do require that you have an interest in these courses, especially, physical chemistry.

Contact Information:
Professor Hans Schelvis' Email: hans.schelvis@nyu.edu

Professor Tamar Schlick

Computational & Biological Chemistry (Theoretical)

General Overview of Research:

The Schlick lab is composed of three separate research groups: the RNA structural biology/bioinformatics group, the DNA structure group, and the DNA Polymerase group. Throughout all of the work pervades a theme of the study of structure/function relationships in nucleic acids through computational modeling. The work of the separate groups is summarized below. We also work closely with leading experimentalists in these areas,from the USA, Europe, Japan, and Israel.

RNA Structure and Function:

It has been increasingly recognized in recent years that small RNA molecules play crucial regulatory roles in many cellular processes. However, the structural/functional repertoire of small RNA molecules has proven to be notoriously difficult to characterize experimentally. Therefore, our RNA group is focused on improving current understanding of RNA's structural repertoire using mathematical modeling and bioinformatics tools. Specifically, our group has pioneered the study of RNA structure design and analysis using mathematical graph theory. One of our goals is to predict novel small functional RNA molecules encoded in genomes through a systematic search and screening for functional motifs. This work is leading to a number of candidate novel RNAs, one of which has been confirmed experimentally. Another goal of our group is to use graph theory and computational techniques to improve the experimental process of in vitro selection of functional RNA molecules through computational design and modeling of RNA sequence pools. We pursue these goals in close collaboration with experimentalists in the areas of genomics neurobiology and RNA synthesis.

Chromatin Folding and Organization:

The DNA group currently studies how the global structure of chromatin (gene packing organization) is altered by environmental changes (such as salt concentrations) and nucleosome modifications (such as histone variations, post-translational modifications, and ATP-dependent remodeling). Our main methods of analysis include Brownian dynamics using macroscopic models. Our macroscopic model represents the rigid nucleosomal core as an irregular surface with discrete charges, the flexible nucleosomal histone tails as protein beads, and the linker DNA as DNA beads. The model incorporates electrostatic interactions, excluded volume interactions, and elastic interactions.

DNA Polymerase Mechanisms:

Human DNA is under constant attack from various endogenous and exogenous agents (e.g., UV light, chemicals, etc.); some of them are potentially harmful. If the damaged DNA is replicated, this can lead to cancer (skin, colon, or lung) and premature aging. Cells have therefore devised an efficient quality control system to repair damaged DNA. One of the most important components of this repair machinery, which the polymerase group is devoted to studying, is the polymerase beta protein enzyme that fills small gaps in the damaged DNA. Polymerase beta helps to discriminate correct from incorrect complementary nucleotide units. During the process of base selection, polymerase

changes conformation (shape); this is thought to happen only when proper base complements are matched to one another. Because of its extreme biomedical importance, polymerase beta has attracted the attention of many experimental scientists. Although exciting progress has been made, many questions remain unanswered. Why do some base pairs escape the repair machinery? How do particular mismatches affect polymerase beta? Recently, our group has begun to study other DNA polymerases, such as polX and Dpo4, which are error prone. Low fidelity polymerases, such as Dpo4, can eliminate stalling at lesions, but make more mistakes in incorporating correct base-pairs during DNA replication compared to polymerase beta. Due to limited structural information, it is not clear if Dpo4 undergoes induced-fit conformational changes like high fidelity polymerases. Our simulations and modeling studies so far have begun to decipher the dynamical pathway of Dpo4. We find startling differences in the motions of Dpo4 in comparison to polymerase beta that might help explain the error-prone nature of low-fidelity enzymes. To study these aspects of polymerase function, our group uses advanced computer simulation approaches to follow the evolution of changes in the conformation of the DNA polymerase in the presence of different nucleotides. Through our efforts, we have laid down in atomic details the sequence of events during polymerases' conformational changes and the protein-DNA interactions that might help the polymerases select the
correct base.

Responsibilities of an Undergraduate Researcher:
The Schlick lab welcomes undergraduate students from diverse fields and encourages them to be independent researchers and thinkers. Many undergraduates are responsible for their own research projects. In this way, the student can truly contribute their own original work to the overall research goals of the lab (as opposed to having only the responsibility of stocking the refrigerators). At the same time, if students are not ready to take on a project of their own, there is always room for them to help out on a project that has already been started.

Availability Requirement for Undergraduates:
The amount of time necessary for research generally depends on what the student wants to get out of the work. A student who wants to begin and finish a project of their own will generally have to devote a lot of time to research. Since studies take up most of people's time during the academic year, it is usually most productive to work in the lab as a full-time researcher over the summer. But it is still possible to get a good body of work done through the school year. One advantage of working in a computational lab is that the researchers have more time control than in experimental "wet" labs, and often times, work can be done at home or any location with proper computing facilities..

Course / Previous Experience Requirements for Undergraduates:
Our lab includes researchers that range from a research professor, to high school students. An eager student will choose a productive avenue of research, regardless of their level of background in computational chemistry or mathematical biology. That being said, knowledge that is most useful includes: mathematics (calculus, probability, statistics), computer programming, chemistry (especially physical), and biology (especially molecular and cellular). At least, it is desirable that students have taken introductory courses in biology or chemistry, and have rudimentary mathematical

abilities. Still, all members of the Schlick group are very helpful, both in general research advice as well as mundane problems. Ultimately, it is most important to have enthusiasm and interest in the work, the ability to communicate progress to other group members as well as the ability to work in a team environment, and especially, a willingness to learn and put in a good amount of effort.

Contact Information:
Professor Tamar Schlick's Email: schlick@nyu.edu

Professor David Schuster

Organic Chemistry & Nanoscience (Experimental)

General Overview of Research:
We are working on synthesizing new types of electron donor-acceptor materials based on fullerenes (C60) with very unusual architectures. These include knotted structures (i.e., catenanes and rotaxanes) as well as molecular wires. We also prepared compounds which are potential inhibitors of HIV protease.

Responsibilities of an Undergraduate Researcher:
My present group includes 4 active undergraduates and 2 PhD students, with 2 additional undergrads in the wings, and one high school student. These students mainly do synthesis, much of it quite demanding, and spectral analysis, and also fluorescence studies, which are critical to these projects. The enzyme inhibition studies are done by a collaborator at Emory University Medical School on samples prepared in my lab.

Availability Requirement for Undergraduates:
I only take on undergrad research students who are willing to make a major commitment of time and effort, which means whatever time they have beyond class and other commitments. Large blocks of time are necessary, e.g., afternoons into the evening, weekends. This type of work can not be done in short time periods. Students must be able to attend weekly group meetings on Wednesdays at 4 PM, where all students participate through presentations and discussions.

Course/Previous Experience Requirements for Undergraduates:
I prefer students who have completed Organic Chemistry, preferably with A grades, although occasionally I take on students current doing Orgo, but only if they are doing well and are committed.

Additional Information:
I encourage my students to make presentations at national meetings, with grant and CAS support. For example, most if not all of my present group will present papers at the Electrochemical Society Meeting in Quebec next May as part of the Fullerene Symposium. Many recent papers from my lab have undergrad students as coauthors.

Recent former undergrads from my group are now in graduate school at Harvard (NSF Fellowship), MIT (Hertz Foundation Fellowship), UCLA (2, one an ACS Organic Division Fellow), and Caltech (Chem Engineering). Another, Phil Baran, now Assistant Professor at Scripps, is one of the brightest stars in the area of synthetic organic chemistry.

Contact Information:
Professor David Schuster's Email: david.schuster@nyu.edu

Professor Nadrian C. Seeman

Nanoscience/Biophysical Chemistry/Biological Chemistry (Experimental)

General Overview of Research:
We work on DNA nanotechnology. We make objects, lattices, devices and materials out of DNA; we also do a little DNA-based computation. The DNA is all synthetic. Check us out at http://seemanlab4.chem.nyu.edu.

Responsibilities of an Undergraduate Researcher:
After a short training period, an undergraduate would take on a small project under direction.

Availability Requirement for Undergraduates:
About a day/week.

Course/Previous Experience Requirements for Undergraduates:
No prior experience; we sometimes work with high school students.

Contact Information:
Professor Seeman's Email: ned.seeman@nyu.edu

Professor Mark Tuckerman

Computational & Quantum Chemistry (Theoretical)

General Overview of Research:

Responsibilities of an Undergraduate Researcher:

Availability Requirement for Undergraduates:

Course/Previous Experience Requirements for Undergraduates:

Contact Information:

Professor Marc Walters

Inorganic Chemistry

General Overview of Research:
The research in the Walters lab is focused on two principle areas. The first of these areas is the synthesis of bio-inspired model compounds of iron-sulfur proteins. Our models as designed to mimic non-covalent interactions between peptide groups and the sulfur atoms of the active site. It is interactions of this type that allow us to design

functional molecules whose properties mimic those of the protein. Our principal tool are surfactants that form reverse micellar structures that in which iron-sulfur complexes are contained in a cavity lined with peptide mimic amide groups that anchor the complexes through hydrogen bonding. We synthesize surfactants that are ideally suited to form host-guest hydrogen bonds.

A second area of research is the synthesis of sulfur compounds (i) as chelators for metals and (ii) as reagents for the detection of chemical warfare agents. One product of this research is an iron reagent for the formation of cyclic disulfides from α,ω-dithiols (e.g. 1,3 propanedithiol).

Responsibilities of an Undergraduate Researcher:
The projects described above are in the capable hands of undergraduates. Junior undergraduate students in my laboratory function at the level of graduate students and have the responsibility of researching their project and optimizing synthetic and spectroscopic protocols. One hallmark of student work is independence. My lab is most suitable for students who prefer primary responsibility for the success of their projects. Guidance is provided by the professor. However a significant degree of independence is expected of the student.

Availability Requirement for Undergraduates:
At the entry level students will need about 10 hours per week for research. At the more senior level students should plan for 15 to 20 hours per week depending on the project.

Course / Previous Experience Requirements for Undergraduates:
The entry level for students in my lab is the end of freshman year. Under extraordinary circumstances Prof. Walters will consider training students at an earlier stage of their study.

Contact Information:
Professor Walter's Email: marc.walters@nyu.edu
Office: 553 or 555 Brown
Office Telephone: (212) 998-8477
Lab Telephone: (212) 998-8494

Professor John Zhang

Computational & Quantum Chemistry (Theoretical)

General Overview of Research:
Research in Prof. John Zhang's computational chemistry group aims to develop and apply theoretical methods to quantitatively determine the energy, structure, and dynamics of molecular systems that are of chemical and biological interest. Currently, our research is primarily focused on following projects:

1. Development and application of the SVRT (semirigid vibrational rotor target) model for general and accurate time-dependent quantum wavepacket computation of elementary chemical reactions such as $OH + CH_3 \leftrightarrows O + CH_4$.

2. We recently developed an efficient MFCC (molecular fractionation with conjugate caps) method to compute protein-ligand, DNA-ligand or other large molecular interaction energies fully *ab initio*. Using the MFCC method, interaction energies of practical protein-ligand systems with thousands of atoms can now be routinely computed by quantum chemistry methods.

3. Application of molecular dynamics and statistical mechanics to the studies of biomolecular interactions and free energy calculations.

4. We are developing a new approximation quantum mechanical approach, namely, MFCC-Assembled Density Matrix (MFCC-ADM), to study the electronic properties of large biomolecular systems such as proteins and nuclear acids.

Responsibilities of an Undergraduate Researcher:
Responsibilities and specific project will be assigned after interview.

Availability Requirement for Undergraduates:
About 10 hours per week

Course/Previous Experience Requirements for Undergraduates:
Calculus, Physical Chemistry I(quantum chemistry), at least one programming language, Organic Chemistry, Biochemistry

Contact Information:
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Office: 1001K

To learn more about Project 1 contact:
Graduate student Qian Cui (qc207@nyu.edu, Rm1002)
To learn more about Project 2 contact:
Graduate students Dawei Zhang (dz266@nyu.edu, Rm 1001R) and Aimin Gao (ag746@nyu.edu, Rm1002)
To learn more about Project 3 contact:
Graduate student Ju Bao (jb1221@nyu.edu, Rm 1002)
To learn more about Project 4 contact:
Graduate student Xihua Chen (xihua.chen@nyu.edu, Rm1002)

Professor Yingkai Zhang

Computational Chemistry (Theoretical)

General Overview of Research:
Prof. Yingkai Zhang's group is interested in developing and applying computational and theoretical methods to investigate chemical reactions in biological systems. Research in this field deepens our understanding the inner workings of biological processes, and will facilitate significant advances in medicine and technology.

Responsibilities of an Undergraduate Researcher:

We invite bright, dedicated undergraduates to join us in this exciting interdisciplinary research. The possible projects range from computational studies of chemical reactions to implementation/test of computational methods, which will be designed based on the students' background, interest and experience.

Availability Requirement for Undergraduates:
The amount of time necessary for this kind of research is 15 hours or more per week.

Course/Previous Experience Requirements for Undergraduates:
A background that includes multivariate calculus, physical chemistry, and some familiarity with computing is ideal, but all applicants will be considered.

Contact Information:
Interested students should send an e-mail Professor Zhang with your current CV and the following information: 1. Prior and current chemistry, physics and math classes. 2. Computing experience.
Professor Yingkai Zhang's Email: yingkai.zhang@nyu.edu