

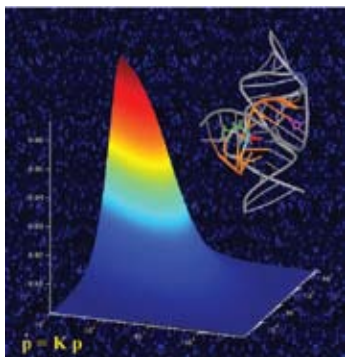
University of Michigan
DEPARTMENT OF CHEMISTRY

PHYSICAL CHEMISTRY

Graduate Program



Physical Chemistry at Michigan has grown dramatically over the last decade, expanding into cutting-edge areas of single molecule spectroscopy, atomic scale imaging, solid state NMR, X-ray spectroscopies, and femtosecond dynamics and multidimensional spectroscopy. The inclusive nature of chemistry as a central science and the importance of a firm theoretical foundation leads to exploration in a diverse range of areas. A selection of these are described below.

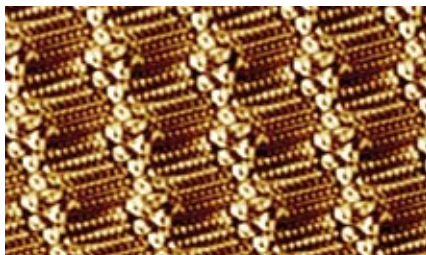


Kinetic rate landscape (left) of an RNA enzyme (right) analyzed by single molecule microscopy (background image). N. Walter

Biophysical Chemistry

Biophysical Chemistry seeks to measure, describe and explain physical phenomena in biological systems at the molecular to supramolecular level. Research in Biophysical Chemistry is highly interdisciplinary in nature and uses a wide variety of spectroscopic techniques on a broad selection of biological systems including both proteins and nucleic acids. At Michigan, particular interests include: Single-molecule and ensemble fluorescence of enzymes; Microscopy of RNA enzymes and of nano-devices; Solution and solid-state nuclear magnetic resonance (NMR) spectroscopy spectroscopy of RNAs, peptides, proteins, and membranes;

X-ray absorption spectroscopy of metallo-enzymes; Mass spectrometric analysis of protein expression in normal and diseased cells; Intracellular chemical dynamics; and computer simulations of complex systems.



STM image of a nanopatterned surface decorated with clusters of aromatic rings spaced by alkane chains. A. Matzger

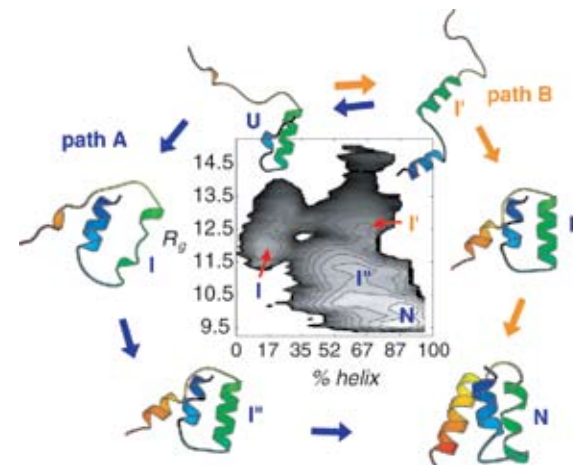
Surface & Nano-Science

The chemistry of surfaces and interfaces is profoundly important in modern science and engineering. Current research in the Chemistry Department involves developing molecular-level understanding of interfaces of prime importance in modern catalytic and electronic materials, biological systems, and drug delivery. Selected examples include the role of surfaces in novel chemotherapy agents, interactions between proteins and polymer surfaces related to biocompatibility of polymers and marine biofouling, membrane protein structure and polymer adhesion, crystallization phenomena in two and three dimensions, hydrocarbon oxidation on metal surfaces, and surface science of chemical sensors. The state-of-the-art techniques applied include sum frequency generation vibrational spectroscopy, atomic force microscopy, scanning tunneling microscopy, X-ray photoelectron spectroscopy, surface infrared spectroscopy, low-energy electron diffraction, mass spectrometry, confocal and resonance laser trapping microspectroscopy, and fluorescence yield near-edge spectroscopy.

Theoretical Chemistry

Theoretical and computational studies play an important role in shaping modern chemistry. Research in the department develops new computational techniques and applies established methodology to address a wide range of systems for molecular electronics, photochemical processes, molecular assembly, biomolecular machines, protein folding, enzymatic catalysis, and drug design. Ongoing research projects use the following:

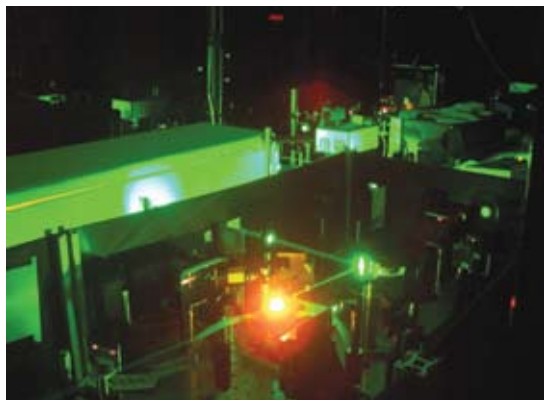
- (1) Statistical mechanics, molecular dynamics, and Monte-Carlo simulations;
- (2) Multi-scale modeling;
- (3) Docking, scoring, and data-mining techniques;
- (4) Advanced electronic structure methods, such as time-dependent density-functional theory (TDDFT);
- (5) Quantum Mechanics Molecular Mechanics (QM/MM) calculations;
- (6) Simulation of quantum molecular dynamics in condensed phase systems;
- (7) Theory of single molecule kinetics and spectroscopy.



Protein folding typically occurs via multiple pathways when viewed at an atomically detailed level. In the figure, the folding progress for the small three-helical bundle protein - fragment B1 of staphylococcal protein A - as computed using detailed molecular dynamics simulations with umbrella sampling statistical mechanical methods is illustrated. The folding free energy landscape for this protein shows folding via two distinct pathways for helix formation versus compaction (as measured by the radius of gyration, R_g). C. Brooks

Spectroscopy

Modern spectroscopies provide powerful tools for studying and manipulating chemical reactions, for investigating molecular materials, and for probing nano-scale systems. Research at the University of Michigan ranges from the study of atmospheric reactions, where physical conditions cover extreme ranges of pressure and temperature, to the use of the worlds smallest light source for optical and spectral imaging on the nanometer scale. Spectroscopic methods of characterization are used in the study of non-crystalline materials including photo-conducting polymers, inorganic-organic composites, molecular aggregates and nanoparticles.



Femtosecond Optics

Femtosecond lasers have many applications in chemistry. At Michigan lasers are used to investigate chemical reactions in condensed phase molecular systems, where relaxation processes on ultrafast time scales control dynamics; to investigate energy and charge transport in novel organic materials, potential candidates for optical limiters, light-emitting devices, and artificial light harvesting; and to control chemical reactions using the interaction between designer light pulses, having precisely controlled phase and amplitude, and the molecular system.

Life in Ann Arbor

The University of Michigan offers a rich intellectual environment. Opportunities for research and collaboration in physical chemistry are enhanced by



top-ranked programs in engineering, physics, applied physics, and biophysics. The University is located in Ann Arbor, a small city of 110,000, combining the comfort and charm of a college town with the vivid cultural life of a large city.

Further Information

For more information about specific research interests see www.umich.edu/~michchem or contact a faculty member directly:

Hashim Al-Hashimi	hashimi@umich.edu
Mark Banaszak Holl	mbanasza@umich.edu
John R. Barker	jrbarker@umich.edu
Charles L. Brooks III	brooksc1@umich.edu
Heather A. Carlson	carlsonh@umich.edu
Zhan Chen	zhanc@umich.edu
Barry D. Dunietz	bdunietz@umich.edu
Eitan Geva	eitan@umich.edu
Theodore Goodson	tgoodson@umich.edu
Raoul Kopelman	kopelman@umich.edu
Kevin Kubarych	kubarych@umich.edu
Adam J. Matzger	matzger@umich.edu
James E. Penner-Hahn	jeph@umich.edu
A. Ramamoorthy	ramamoor@umich.edu
Roseanne J. Sension	rsension@umich.edu
Nils G. Walter	nwalter@umich.edu

How to Apply

Application to the Chemistry Graduate Program at the University of Michigan is online at www.umich.edu/~michchem/graduate/

For questions regarding admission see www.umich.edu/~michchem or contact the department by

Website:	www.umich.edu/~michchem
Email:	ChemAdmissions@umich.edu
Phone:	toll free 888-999-2436 or 734-764-7278
Fax:	734-647-4865

cover: Optical parametric oscillator for producing tunable femtosecond pulses.

Chemistry at the University of Michigan

Physical Chemistry

