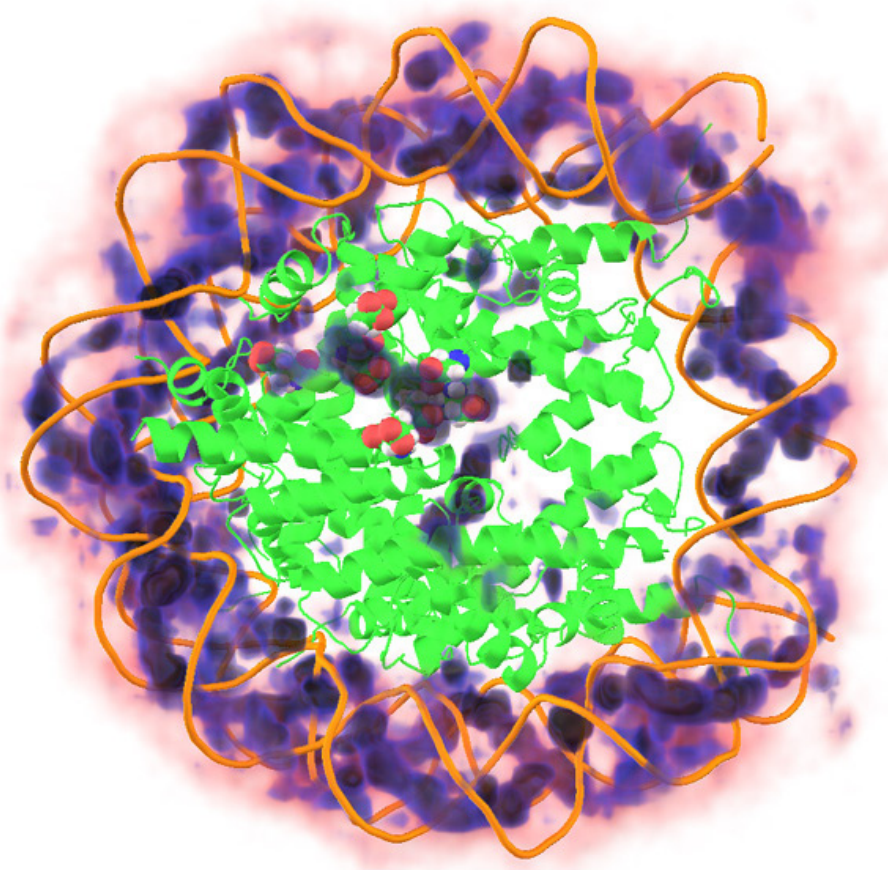


THEORETICAL CHEMISTRY FACULTY

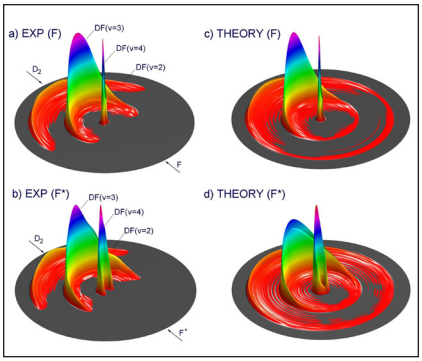
UNIVERSITY OF MARYLAND

MILLARD ALEXANDER
Distinguished University Professor

BA (Magna Cum Laude) in Chemistry, Harvard College, 1964; PhD Université Paris-Sud (with High Distinction), 1967; Research Fellow, Harvard University 1967-71; University of Maryland (1971-present) and Institute for Physical Science and Technology (1999-present); Distinguished University Professor, University of Maryland (1999-present).

NSF Predoctoral Fellow 1964-1967; Outstanding Young Teacher Award, D.C. Institute of Chemists 1977; Elected Fellow, American Physical Society 1984; Alexander von Humboldt Foundation, Senior US Scientist Award 1989; Excellence in Teaching Award, University of Maryland 1992; Contribution to Science Award, Sigma Xi 1993; Hillebrand Award, American Chemical Society 1996; Dr. Lee's Visiting Research Fellowship, Christ Church, Oxford, UK 1997; John Simon Guggenheim Memorial Fellowship 1997; Kirwan Faculty Research and Scholarship Prize, University of Maryland 1999.

Alexander's research has provided a framework for the understanding of non-adiabatic effects in molecular collisions, in weakly bound complexes and in molecular photodissociation. By combining state-of-the art techniques in *ab initio* quantum chemistry and new methods in quantum collision theory, he has pushed forward the frontier in the understanding of how electronic and nuclear motion is coupled in elementary inelastic and reactive collisions. Alexander's earlier work on inelastic scattering of open-shell molecules enabled the understanding of a wide variety of subsequent experimental studies on these systems.



Comparison between differential cross sections for the reaction of F/F with D_2 predicted by Alexander's calculations and by crossed molecular-beam scattering studies by Yang and co-workers in Dalian (PRC).*

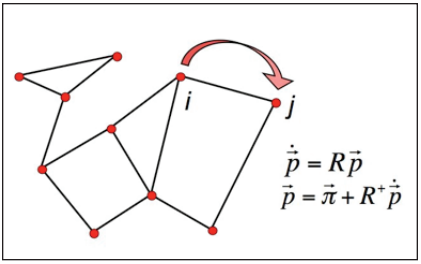
CHRISTOPHER JARZYNSKI
Professor

AB Princeton University 1987; Fulbright Scholar, Warsaw, Poland, 1987-88; PhD University of California, Berkeley 1994; Research Associate, Institute for Nuclear Theory, Seattle 1994-96; Director-Funded Postdoctoral Fellow, and Technical Staff Member, Los Alamos National Laboratory 1996-2006; Department of Chemistry and Biochemistry, and Institute for Physical Science and Technology, University of Maryland, College Park 2006-present.

Raymond and Beverly Sackler Prize in the Physical Sciences 2005; Fellow American Physical Society 2009.

Recent years have seen tremendous technological advances in the ability to observe and manipulate individual molecular systems that exhibit mechanical motion. Together with theoretical modeling and numerical simulation, this progress has revealed how biomolecular machines carry out sophisticated assignments such as the replication of DNA, and has spurred the first steps toward the synthesis of artificial molecular complexes that are similarly capable of harnessing energy to perform useful tasks. These tiny machines pose a challenge to theorists: how do the laws of thermodynamics apply to nanoscale systems, where thermal fluctuations dominate? In my group, we develop theoretical tools for understanding nonequilibrium behavior, and computational methods for estimating thermodynamic properties; and we construct and analyze models that provide insight into complex phenomena.

Current research: (1) application of identities from equilibrium and nonequilibrium statistical mechanics to develop efficient methods for estimating free energies, and for sampling systems with complex energy landscapes such as biomolecules; (2) investigation of universal laws that characterize the fluctuations of microscopic systems far from thermal equilibrium; (3) development of a systematic framework for the understanding and design of artificial molecular machines; (4) analysis of model systems that elucidate the relationship between thermodynamics and information processing in nanoscale systems.



A simple mathematical model of a microscopic machine, with the states of the molecular complex represented as points, and possible transitions as edges.

GAREGIN PAPOIAN
Monroe Martin
Associate Professor

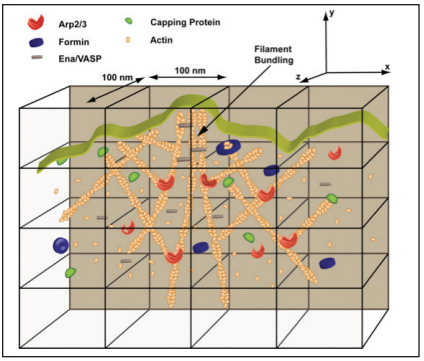
Russian Academy of Sciences, Higher Chemical College 1990-1994; PhD Cornell University 1999; Postdoctoral Fellow, University of Pennsylvania 2000, and University of California San Diego 2001-2004; Assistant Professor, University of North Carolina at Chapel Hill 2004-2010; Monroe Martin Associate Professor, Department of Chemistry and Biochemistry and Institute for Physical Science and Technology, University of Maryland, 2010-present.

Phillip and Ruth Hettleman Prize for Artistic and Scholarly Achievement 2010; ACS Hewlett-Packard Outstanding Junior Faculty Award 2010; National Science Foundation CAREER Award 2009; Camille Dreyfus Teacher-Scholar 2008; Beckman Young Investigator 2007; Camille and Henry Dreyfus New Faculty Award 2004; National Institutes of Health Postdoctoral Fellowship 2001.

My group uses theoretical physical chemistry techniques, including advanced computational methods, to study biological processes at multiple scales, from single protein functional dynamics and chromatin folding and stability to cell-level processes, such as cell motility:

1) Cell motility plays a key role in human biology and disease, contributing ubiquitously to such important processes as embryonic development, wound repair and cancer metastasis. Our research aims to elucidate the physical chemistry behind these complex, far-from-equilibrium mechano-chemical processes.

2) We also aim to understand the way DNA is packaged in the nuclei of higher organisms. The total length of DNA in each eukaryotic cell can reach 2 m, however, it must be housed in a micrometer size cell. This staggering six orders of magnitude compaction is achieved by wrapping DNA around protein octamers called histones, which then further fold into higher order chromatin structures. Misregulation of chromatin may result in human genetic diseases. Our group develops physico-chemical computational models to study the chromatin folding and dynamics.



Complex physical and chemical processes govern motility of eukaryotic cells. Polymerization and dynamical remodeling of the actin network depend on a delicate interplay between mechanical forces, numerous chemical reactions, and molecular transport.

ROSS SALAWITCH
Professor

BS Cornell University 1981; PhD Harvard University, 1987; Postdoctoral Fellow and Research Associate, Harvard University 1988-1994; Research Scientist, NASA Jet Propulsion Laboratory 1994-2007; Visiting Faculty Associate, California Institute of Technology 2005-2007; Department of Chemistry and Biochemistry, Department of Atmospheric and Oceanic Science, and Earth System Science Interdisciplinary Center, University of Maryland 2007-present.

Highly Cited Researcher in Geosciences 2003 to present; American Geophysical Union Yoram J. Kaufman Award for Unselfish Cooperation in Research 2009; NASA Exceptional Achievement Medal, 1999 and 2007.

We develop computer models to quantify the impact of human activity on atmospheric composition, with a focus on stratospheric ozone depletion and recovery, air quality, climate change, and the global carbon cycle. Our studies are data intensive: we participate in atmospheric chemistry field campaigns such as TC4 (Costa Rica, 2007), ARCTAS (Alaska, 2008) and Discover-AQ (Eastern US, 2011) and we routinely use data from satellite missions, such as the NASA Aura experiment. We examine interactions between various disciplines of atmospheric chemistry, such as how a warmer future climate driven by rising levels of greenhouse gases may lead to higher levels of harmful surface ozone; how actions presently being taken to reduce the emission of precursors of harmful aerosols may accelerate future warming of climate; and, how the eventual recovery of the beneficial stratospheric ozone layer, due to the ban on emission of CFCs and related compounds, might be altered by climate change. Salawitch is a member of the NASA Orbiting Carbon Observatory-2 science team that is building an instrument, scheduled for launch in February 2013, designed to revolutionize our understanding of the global carbon cycle. Also, he is a regular participant in the authorship of Scientific Assessment of Ozone Depletion Reports issued every four years by World Meteorological Organization/ United Nations Environment Programme.

Data from the NASA Aura satellite is used by Salawitch's group to assess the impact of halogens on ozone. Image courtesy of Northrop Grumman Corporation.

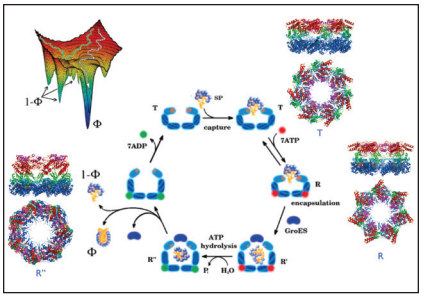
DEVARAJAN THIRUMALAI
Distinguished University Professor

BS Indian Institute of Technology Kanpur 1977; PhD University of Minnesota 1982; Post-Doctoral Fellow, Columbia University 1982-1985; Director, Biophysics Program, University of Maryland 2005-present. Editorial Board, *J. Chemical Physics* 2008-present; Editorial Board, *Protein Evolution, Design, and Selection*, 2005-present. Served on the editorial boards of *Theoretical Chemistry Accounts* and *Communication chein Mathematical Methods*.

Camille and Henry Dreyfus Foundation 1985-1987 & 1990; Distinguished New Faculty Award 1985; Alfred P. Sloan Fellowship 1986-1988; Presidential Young Investigator Award 1987-1992; Outstanding Junior Faculty Award 1989; Maryland Outstanding Young Scientist 1995; Distinguished Faculty Research Fellowship Award 1998.

The Thirumalai group uses theoretical methods in statistical mechanics, soft matter science, and computer simulation methods to study wide-ranging problems in biology. Currently we are focusing on the following research areas:

(1) After making fundamental contributions in understanding how proteins and RNA fold, our group is focusing on how aberrant folding of proteins can give rise to formation of amyloid fibrils, which are linked to a number of neurodegenerative diseases. (2) Increasing focus on how to describe RNA and protein folding occurring under crowded cellular conditions using theoretical concepts in polymer and colloid science. (3) Developing theories to predict the outcomes of single molecule force spectroscopy of cell adhesion complexes and signaling proteins. In this area both conceptual issues on the meaning of measurements as well as applications are being addressed. (4) New computational models of biological nanomachines such as bacterial chaperones (in collaboration with George Lorimer), molecular motors, and RNA polymerases are being used to describe their functions. In all these areas our research group works closely with experimentalists worldwide.



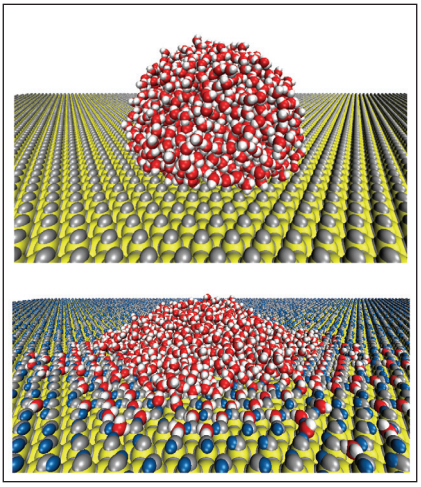
Iterative annealing mechanism describing the function of a biological machine, the bacterial chaperonin GroEL. Figure shows how allosteric transitions of GroEL and annealing of proteins is coupled.

JOHN WEEKS
Distinguished University Professor

BA (Magna Cum Laude) in Physics, Harvard College, 1965; PhD in Chemical Physics, University of Chicago, 1969; Postdoctoral Research Associate, University of California San Diego 1969-71 and Cambridge University 1971; Member Technical Staff, Bell Laboratories, 1972-1990; Professor, Institute for Physical Science and Technology, and Department of Chemistry and Biochemistry, University of Maryland 1990-1995; Distinguished University Professor, University of Maryland 1995-present.

Member, National Academy of Sciences; Fellow, American Academy of Arts and Sciences; Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids; Fellow, American Physical Society.

The Weeks group uses methods of statistical mechanics to study static and dynamic properties of solid surfaces and properties of non-uniform and confined liquids, particularly those with long-ranged Coulomb and dipolar interactions. The surface work interfaces closely with experiments carried out by Professor Janice Reutt-Robey and other members of the Materials Science Research and Engineering Center at Maryland. We study in particular theories of crystal growth and dynamical properties of steps and islands on crystal surfaces. Water and ions in non-uniform environments play a key role in a host of biophysical and materials systems. We are developing new and general theories describing effects of the long-ranged Coulomb interactions. Current applications include properties of water at hydrophobic and hydrophilic surfaces, solvation of charged colloids in ionic fluids and water, effects of counterions on the folding of charged polymers, and how to treat Coulomb interactions in coarse-grained models of complex systems.



Water droplets on model hydrophobic and hydrophilic silica surfaces determined by molecular dynamics simulations using the extended simple point charge model.

Theoretical Chemistry at the University of Maryland

MICHAEL P. DOYLE

The Department of Chemistry and Biochemistry

at the University of Maryland has exceptional strength in theoretical chemistry, with research focusing on innovative development of new methods, the elaboration of new computational algorithms, and large-scale computer modeling of systems of key importance to chemistry. The faculty members in theoretical chemistry (Alexander, Jarzynski, Papoian, Salawitch, Thirumalai, and Weeks) are international leaders in their subdisciplines and excel in these areas. Their contributions to science have been recognized by major professional awards, including a John Simon Guggenheim Memorial Fellowship, the Joel Hildebrand Prize of the American Chemical Society, and the Raymond and Beverly Sackler Prize; and John Weeks is a member of the National Academy of Sciences and the American Academy of Arts and Sciences.

The University of Maryland provides an environment for discovery and innovation in the chemical sciences. Experimental and computational chemistry are interlinked in unique ways that often provide basic insights that are not revealed by experiment or theory alone. Research groups are integrated with other departments or institutes, including the Institute for Physical Science and Technology, to provide broad exposure to the challenging problem that confronts science and society today.

Michael P. Doyle, Chair
Department of Chemistry and Biochemistry

UNIVERSITY OF MARYLAND

Department of Chemistry and Biochemistry
University of Maryland
College Park, MD 20742-4454
www.chem.umd.edu