# Free Radicals & Phi Lambda Upsilon

## Research Panel

March 2, 2011
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**Professor David Masiello**
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Teaching: Teaches classes from 1$^{st}$-year to graduate level; developed 3 new undergraduate classes.
Research Areas: Inorganic, organometallic, bioinorganic and physical organic chemistry, with emphasis on fundamental understanding of redox processes and proton-coupled electron transfer.
We aim to elucidate experiment in nanoscale optics and plasmon-enhanced molecular spectroscopy using first-principles theory and computation. Well-defined descriptions of such phenomena, which involve the simultaneous interaction of molecules, nanoscale plasmon-supporting metals, and the electromagnetic field, are difficult to formulate because of the widely varying length scales over which the relevant chemical and physical processes occur. We accomplish this task by carefully blending together molecular-electronic propagator methods as well as explicitly time-dependent descriptions of quantum molecular dynamics coupled to the continuum-electrodynamics of the field and metal. We also employ purely classical electromagnetic theory to describe nanoscale metal structures and their interaction with light. Development of the software necessary to explore each of these theoretical concepts is an essential aspect of our research as we work in areas where no black-box applications exist.

**Professor D. Michael Heinekey**
Department of Chemistry
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Professional Preparation:
Postdoctoral Fellow, UC Berkeley, Berkeley, CA, 1982-1984 (Earl Muetterties)
Ph.D., University of Alberta (W. A. G. Graham), 1982; B.Sc., University of Victoria, 1977
Research Interests: Homogeneous catalysis, $H_2$ complexation, $H_2$ storage, energy conversion
Selected Recent Publications:

Steven L Matthews and D. M. Heinekey "A Carbonyl-rich Bridging Hydride Complex Relevant to the Fe-Fe Hydrogenase Active Site" *Inorganic Chemistry,*2010, *49*, 9746.

Jonathan D. Egbert and D. M. Heinekey "Dihydrogen Complexes of the Chromium Group: Synthesis and Characterization of $(Arene)M(CO)_2(H_2)$ Complexes.*" Organometallics* 2010, *29*, 3387.

Travis J. Hebden, Karen I. Goldberg, Alan S. Goldman, K. Krogh-Jespersen, Thomas J. Emge and D. M. Heinekey, "Dihydrogen/Dihydride or Tetrahydride? An Experimental and Computational Investigation of Pincer Iridium Polyhydrides" *Inorganic Chemistry*, 2010, *49*, 1733

G. J. Kubas and D. M. Heinekey "Activation of Molecular Hydrogen" Invited review chapter for *Physical Inorganic Chemistry*: *Reactions, Processes and Applications.* John Wiley & Sons, 2010

Joseph Meredith, Karen I. Goldberg, Werner Kaminsky and D. M. Heinekey, "Dinuclear Iridium Complexes Containing $Cp^*$ and Carbonyl Ligands: Synthesis, Structure and Reactivity"*Organometallics,* 2009, *28*, 3456

D. M. Heinekey "Hydrogenase Enzymes: Recent Structural Studies and Active Site Models."*J. Organomet. Chem.* 2009, *694*, 2671

Serena Fantasia, Jonathan D. Egbert, Heiko Jacobsen, Luigi Cavallo, D. M. Heinekey and Steven P. Nolan. "Activation of $H_2$ by Palladium (0): Formation of the Monomeric Dihydride Complex *trans* $[(IPr)(PCy_3)Pd(H)_2]$" *Angewandte Chemie*, 2009, *48*, 5182

Inigo Aguirre De Carcer and D. M. Heinekey "Synthesis and Characterization of Sulfur Rich Iron(II)

**Professor James M. Mayer**
Department of Chemistry
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Research in Professor Mayer's group is focused on chemical processes that involve transfers of both electrons and protons. These processes span the fields of inorganic, bioinorganic, organometallic, and physical organic chemistry – and are of special interest in energy conversion. Studies in the group range from fundamental examination of basic chemical reaction steps to the development of new catalysts.

Research in the Mayer labs has led to a new, detailed, and predictive understanding of hydrogen atom transfer reactions. These are chemical reactions in which a proton and an electron transfer from one group to another, $AH + B \rightarrow A + HB$. Continuing studies are extending this work to reactions in which the proton and electron transfer to or from different molecules. Such reactions are poorly understood but are probably very common in biochemical processes and in reactions of key importance in the conversion of chemical and electrical energy. A very wide range of current projects in the group fall under this heading, from searching for a new process to convert methane to ethane (relevant to efficient natural gas conversion) to models for ubiquitous enzymatic peroxidase and oxidase reactions. The Mayer group is exploring new catalysts for the reduction of dioxygen ($O_2$) to water – key to new fuel cell technologies – and catalysts for the oxidation of water to $O_2$, which is key to the production of chemical fuels from electricity. Finally, the fundamental proton/electron transfer ideas are being applied to derive new insights in the chemistry of metal oxides, using nanoparticles.

**Professor Frantisek Turecek**
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The Turecek group is currently involved in several lines of research using mass spectrometry as the core technique. A unique tandem mass spectrometer (declared tongue-in-cheek "Seattle's best mass spectrometer" by a local weekly and immortalized in an abstract painting sold to an art collector in Manchester, UK) is used to generate transient neutral intermediates of chemical reactions relevant to the chemistries of the atmosphere, flames, and radiation damage. This research involves ion chemistry, kinetic measurements on the microsecond time scale, laser photoexcitation, isotope labeling, and theory. These studies have recently been expanded to the generation of biologically interesting transient intermediates. An important component of this research relies on high-level quantum chemical calculations including tunnel effects and unimolecular kinetics.

Special instruments for single-cell analysis and ion-surface interactions are the latest addition to the armory of mass spectrometers in the Turecek lab. Soft and reactive landing of proteins is used for dry immobilization on metal surfaces while retaining the protein function, such as enzymatic activity or substrate recognition.

Collaboration with the labs of Professors M. H. Gelb (UW Chemistry and Biochemistry) and R. C. Scott (UW Pediatrics and Seattle Children's Hospital), resulted in the development of multiplex strategies for assaying enzymes and proteomics. Enzymes responsible for genetic diseases in children are studied in cells and dried blood spots and their action quantified by electrospray-ionization mass spectrometry to provide medical diagnosis. This line of research involves a good deal of organic chemistry in combination with instrumental analysis. The developed technologies are applied in newborn screening laboratories in several states (New York, Illinois, Missouri, Washington, New Mexico).

**Other resources for Undergraduate Research:**

- Undergraduate Research Program
  http://www.washington.edu/research/urp/
- UW Undergraduate Research Symposium
  May 20, 2011 in Mary Gates Hall
- Department of Chemistry – Research
  http://depts.washington.edu/chem/chemresearch/