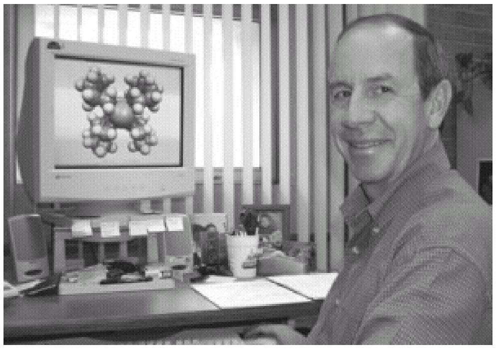
Faculty Profile



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Dennis Lichtenberger

Professor

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Honors

- Galileo Circle Fellow, College of Science, 2012
- Associate Editor, *Organometallics*, 2008-
- Chair-elect and Chair, Organometallic Subdivision of the Inorganic Division of the ACS, 2010-2011
- Ninth Annual University Graduate and Professional Education Teaching and Mentoring Award, 2008
- Coates Lectureship, University of Wyoming, 2006
- Plenary Lecturer, Taller de Quimica Cinvestav, Mexico City, 2004

Education and Appointments

- B.S. 1969, Indiana University, Bloomington
- Ph.D. 1974, University of Wisconsin, Madison
- Postdoctoral 1974-1976, University of Illinois, Urbana-Champaign

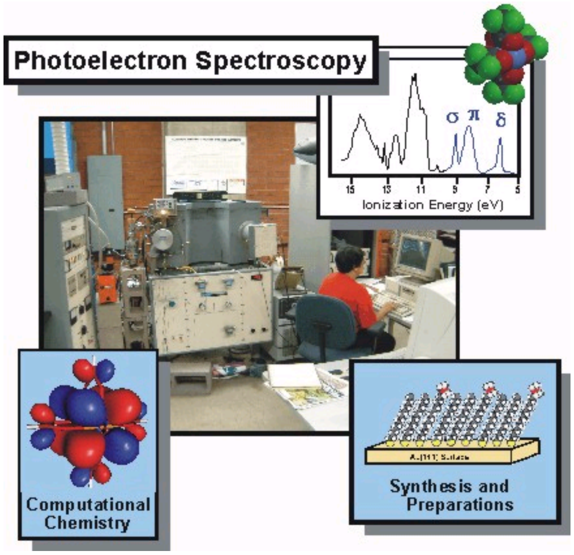
Research Interests

- Inorganic
- "Theory, Modeling, and Simulation"
- Bioinorganic
- Energy Science
- Spectroscopy and Instrument Development
- Surfaces and Solid State
- Synthesis/Synthetic Methods Development

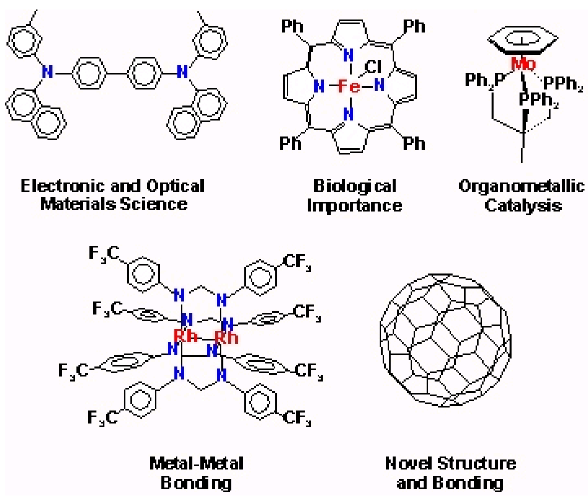
Research Summary

SOLVING ELECTRON MYSTERIES.
Electron Interactions and Transfers in Catalysis, Biology, Materials, and Devices.

This research program encompasses studies of organometallic structure, bonding, reactivity, and catalysis and extends to bioorganometallic chemistry, metal-metal bonding, molecular clusters, and related areas. Most recently this research has moved toward electron transfer processes, molecular electronics, and solar fuels. A central theme of this research has been to probe and understand this chemistry at the level of electronic structure. In one sense, all chemical behavior may be viewed as the movement of electrons. An obvious example is the oxidation and reduction processes of metalloenzymes in biology, but so too is the selective making and breaking of bonds in industrial catalysis, the transport of electrons in molecular wires, and the interactions of molecules with light. Many of the principles of electronic structure and bonding that have been discovered in this research have followed from the development and application of photoelectron spectroscopy, a technique that is often introduced in freshman chemistry texts. Computational chemistry is also an important aspect of this research, and photoelectron spectroscopy is the most direct method to test and validate electron energies in developing computational methods. The special nature or our research methods has led to numerous fruitful and exciting collaborations with scientists from around the world.

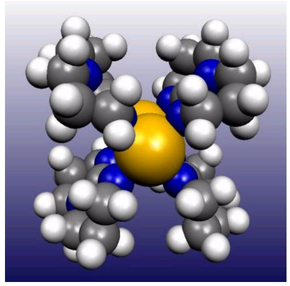


The research as depicted in the figure above offers opportunities in high-resolution gas-phase spectroscopy, ultra-high vacuum surface analysis, computational chemistry, synthesis of new molecules and materials, and/or development of new methods and instrumentation. Students choose the projects in which they are most interested, and may focus on inorganic, physical, analytical, organic, or biological chemistry areas. Examples of chemical systems studied in this research program are shown below:



All chemical behavior involves movement of electrons. Chemical reactivity and catalysis depend on mechanisms that move electrons from existing bonds in starting materials to new bonds in desired products. Movement of electrons in materials is important to electrical conductivity and optical properties for technological applications. In biology, electron transfer involving active metal sites is central to many life processes. This research provides fundamental information for understanding all of these processes - the clues for solving the many mysteries of electron behavior in chemistry.

We are particularly interested in the study of molecules with unusual electronic structure and bonding modes. These molecules offer opportunities for unique properties and new applications. For instance, our discovery of the only molecule that requires less energy to give up an electron than any atom in the periodic table opens a new realm of behavior with many potential applications. The figure below shows the structure of this molecule. The two gold-colored atoms in the center are tungsten atoms, the blue atoms are nitrogens, and the rest is hydrocarbon.



We have developed instrumentation for gas-phase photoelectron spectroscopy of large molecules that is not matched elsewhere. It is the only instrumentation capable of measuring the ionization energies of many important molecules, including the one pictured. As a consequence, we are often the only source of this information for other researchers. In order to serve the needs for this information, we have established an open-access user facility for gas-phase electron spectroscopy. We have numerous rewarding collaborations and often share students with other research groups, both within this Department and in other institutions.

Selected Publications

- Olga Lobanova Griffith, John E. Anthony, Adolphus G. Jones, Ying Shu, and Dennis L. Lichtenberger. Substituent effects on the electronic characteristics of pentacene derivatives for organic electronic devices: dioxolane-substituted pentacene derivatives with triisopropylsilylethynyl functional groups. *J. Am. Chem. Soc.*, 2012, *134* (34), 14185-14194. (http://dx.doi.org/10.1021/ja3056672)
- Michael H. Palmer, Philip J. Camp, Soren Vronning Hoffmann, Nykola C. Jones, Ashley R. Head, and Dennis L. Lichtenberger. The electronic states of 1,2,4-triazoles: A study of 1H- and 1-methyl-1,2,4-triazole by vacuum ultraviolet photoabsorption and ultraviolet photoelectron spectroscopy and a comparison with ab initio configuration interaction computations. *J. Chem. Phys.*, 2012, *136*, 094310 (11 pages). (http://dx.doi.org/10.1063/1.3692164)
- Nicholas J. Wiebelhaus, Matthew A. Cranswick, Eric L. Klein, L. Tori Lockett, Dennis L. Lichtenberger, and John H. Enemark. Metal-Sulfur Valence Orbital Interaction Energies in Metal-Dithiolene Complexes: Determination of Charge and Overlap Interaction Energies by Comparison of Core and Valence Ionization Energy Shifts. *Inorg. Chem.*, 2011, *50*, 11021-11031.(http://dx.doi.org/10.1021/ic201566n)
- Deven P. Estes, Aaron K. Vannucci, Ariel R. Hall, Dennis L. Lichtenberger, Jack R. Norton. Thermodynamics of the metal-hydrogen bonds in(η5-C5H5)M(CO)2H (M = Fe, Ru, Os). *Organometallics*, 2011, *30*, 3444-3447. (http://dx.doi.org/10.1021/om2001519)
- Jaime A. Flores, Jose G. Andino, Nikolay P. Tsvetkov, Maren Pink, Robert J. Wolfe, Ashley R. Head, Dennis L. Lichtenberger, Joseph Massa, and Kenneth G. Caulton. Assessment of the Electronic Structure of 2,2'-pyridylpyrrolides as Ligands. Inorg. Chem., 2011, *50*, 8121-8131. (http://dx.doi.org/10.1021/ic2005503)
- Michael H. Palmer, Soren Vronning Hoffmann, Nykola C. Jones, Ashley R. Head, Dennis L. Lichtenberger. The Electronic States of 1,2,3-Triazole Studied by Vacuum UV Photoabsorption and UV Photoelectron Spectroscopy, and a Comparison with ab initio Configuration Interaction Methods. *J. Chem. Phys.,* 2011, *134*, 084309-321.(http://dx.doi.org/10.1063/1.3549812)
- Jinzhu Chen, Aaron K. Vannucci, Charles A. Mebi, Noriko Okumura, Susan C. Borowski, L. Tori Lockett, Matthew Swenson, Dennis L. Lichtenberger, Dennis H. Evans, and Richard S. Glass. Catalysis of Electrochemical Reduction of Weak Acids to Produce H2: Role of O-H...S Hydrogen Bonding. *Phosphorus, Sulfur and Silicon and the Related Elements*, 2010, *186*, 1288-1292. Invited paper. (http://dx.doi.org/10.1080/10426507.2010.523035)
- Manfred Bochmann, Maurice Brookhart, John A. Gladysz, Dennis L. Lichtenberger, Lanny S. Liebeskind, Tobin J. Marks, Richard R. Schrock, Dwight A. Sweigart, Kenton H. Whitmire. Dedication to the Special Volume for Dietmar Seyferth. *Organometallics,* 2010, *29(21)*, 4647-4647. (http://dx.doi.org/10.1021/om100975m)
- John A. Gladysz, Manfred Bochmann, Dennis L. Lichtenberger, Lanny S. Liebeskind, Tobin J. Marks, Dwight A. Sweigart. Another Great Day for Organometallic Chemistry. *Organometallics,* 2010, *29(22)*, 5737-5737. (http://dx.doi.org/10.1021/om101007r)
- Jinzhu Chen, Aaron K. Vannucci, Charles A. Mebi, Noriko Okumura, Susan C. Borowski, Matthew Swenson, L. Tori Lockett, Dennis H. Evans, Richard S. Glass and Dennis L. Lichtenberger. Synthesis of Diiron Hydrogenase Mimics Bearing Hydroquinone and Related Ligands. Electrochemical and Computational Studies of the Mechanism of Hydrogen Production and the Role of O–H---S Hydrogen Bonding. *Organometallics,* 2010, *29*, 5330-5340. (http://dx.doi.org/10.1021/om100396j)

- Olga Lobanova Griffith, Adolphus G. Jones, John E. Anthony and Dennis L. Lichtenberger. Intermolecular Effects on the Hole States of Triisopropylsilylethynyl-Substituted Oligoacenes. *J. Phys. Chem. C.,* 2010, *114(32)*, 13838-13845.

- Brandi M. Cossairt, Christopher c. Cummins, Ashley R. Head, Dennis L. Lichtenberger, Raphael J.F. Berger, Stuart A. Hayes, Norbert W. Mitzel and Gang Wu. On the Molecular and Electronic Structures of AsP3 and P4. *J. Am. Chem. Soc.,* 2010, *132(24)*, 8459-8465. http://dx.doi.org/10.1021/ja102580d)

- Olga Lobanova Griffith, John E. Anthony, Adolphus G. Jones, and Dennis L. Lichtenberger. Electronic Properties of Pentacene versus Triisopropylsilylethynyl-Substituted Pentacene: Environment-Dependent Effects of the Silyl Substituent. *J. Am. Chem. Soc.,* 2010, *132(2)*, 580-586. (http://dx.doi.org/10.1021/ja906917r)

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- Chen, Shentan; Chisholm, Malcolm H.; Davidson, Ernest R.; English, Jason B.; Lichtenberger, Dennis L. Theoretical and Spectroscopic Investigations of the Bonding and Reactivity of (RO)3M≡N Molecules, where M = Cr, Mo, and W. *Inorg. Chem.* 2009, *48 (3)*, 828-837 (chosen for the cover article). (http://dx.doi.org/10.1021/ic801786u)

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- Felton, G. A. N.; Vannucci, A.K.; Chen, J.; Moser, T.; Okumura, N.; Petro, B.J.; Zakai, U.I.; Evans, D.H.; Glass, R.H.; Lichtenberger, D.L. Hydrogen Generation from Weak Acids: Electrochemical and Computational Studies of a Diiron Hydrogenase Mimic. *J. Am. Chem. Soc.* 2007, *129(41)*, 12521-12530.

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- Lichtenberger, D. "The Electron Distribution, Bonding, and J(Si-H) NMR Coupling Constant in (η5-C5H5)$(CO)_2MnHSiCl_3$: The Molecular Orbital View." *Organometallics* 2003, *22 (8)*, 1599-

1602.

- Lichtenberger, D. L.; Fan, H. -J.; Gruhn, N. E. Ligand-Mediated Metal-Metal Interactions and Localized *versus* Delocalized Mixed-Valence Cation States of Biferrocene and *Bis*(μ-fulvalenediyl) diiron Characterized in the Gas Phase by Valence Photoelectron Spectroscopy. *J. Organomet. Chem.* 2003, *666*, 75-85.
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