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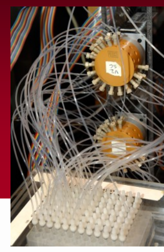

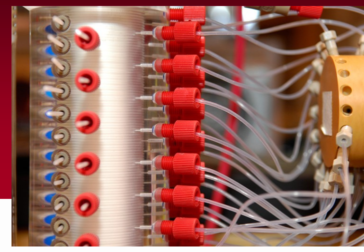

The Gene and Linda Voiland School of

Chemical Engineering and Bioengineering

2014 Seminar Series
Monday, September 29, 2014
12:00 p.m. CUE 319

Michel Dupuis
Physical Sciences Division
Pacific Northwest National Laboratory (PNNL)
Richland, WA

Michel Dupuis is a laboratory fellow at PNNL . His research interests are in the area of computation for chemistry and materials relevant to new energy technologies, in particular the use of multi-scale, multi-physics, and high-performance computing approaches, to gain fundamental understanding that leads to predictive design. Recent fields of application involve energy conversion (catalysis, photocatalysis, photovoltaics) and energy storage (fuel cells, batteries). He was elected as a Member of the International Academy of Quantum Molecular Sciences in 2005, a Fellow of the American Physical Society in 2007, and a Fellow of the American Association for the Advancement of Sciences in 2008 for his contributions to the advancement of the quantum molecular sciences, including the development of high performance computer codes for electronic structure calculations (HONDO, GAMESS, and NWCHEM).

The Power of Computing for Chemistry Fundamentals in New Energy Technologies

Modern multi-scale computation and simulation capabilities allow us to address successfully many of the complex chemistry and physics fundamentals of sun-to-fuel and electricity-to-fuel energy conversions. In this presentation we will describe recent studies relevant to these new energy technologies and highlight successes and areas of challenging new research.

In the context of solar energy conversion, characterization of electron / hole separation, recombination, and transport is essential to design of efficient devices. We successfully characterized the e/h transport properties of TiO_2 and other oxides using density functional theory DFT combined with Marcus/Holstein theory. Our studies led us also to formulate a universal role of excess electrons on the surface chemistry of oxides. In the context of fuel-to-electricity conversion, understanding the factors affecting proton transport in polymeric and ionic liquid membranes of PEM fuel cells is essential toward designing efficient low cost stable membranes. Ab initio and classical molecular dynamics MD combined with percolation theory provided a means to characterize successfully pore structure and proton transport properties. Water percolation is a powerful descriptor characterizing efficient proton transport. Most recently, in the context of electricity-to-fuel conversion our focus has been on molecular electro-catalysis. DFT-based quantum QM and mixed QM/MM approaches coupled with micro-kinetic modeling have led to the accurate characterization of the catalytic performance of novel proton relay-based molecular catalysts for H_2 oxidation and evolution. These efforts have reached what is perhaps an unprecedented level of success that put us within grasp of design by computer.

These studies underscore the power of computation and the impact of high performance computing in characterizing the fundamental chemistry in complex molecular and solid state environments. Successes and challenges point to the key role of high performance and massively parallel computing and the essential need for further advances in methods and computer codes for multi-scale modeling.

Acknowledgements: This research was supported in part by the Center for Molecular Electrocatalysis, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) and in part by DOE/BES Division of Chemical Sciences, Geosciences & Biosciences. Pacific Northwest National Laboratory is operated for the U.S. Department of Energy by Battelle.