

Physics Colloquium

Michigan Technological University

Thursday, October 15, 2009 at 4:00 pm

Room 139 Fisher Hall

Theory and Modeling for Energy Applications: Charge Transport in Complex Molecular and Solid State Environments



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Abstract: In this presentation we will highlight multi-scale investigations of charge transport and reactivity in complex environments, relevant to energy applications. In the first part of our talk we will describe first-principles based studies of (1) e^-/h^+ transport, trapping, and energy redistribution in TiO_2 , (2) surface structure and material dependence of these properties, and (3) detailed reaction mechanisms of oxygenated species, all issues relevant to light-to-chemical energy conversions. In the second part of the talk we will describe multi-scale studies of proton transport in polymeric electrolyte membrane (PEM) relevant to chemical energy-to-electricity conversions. This work makes use of modern computational methodologies in DFT and ab initio and classical molecular dynamics MD from the molecular scale to the meso scale.

Biography: Dr. Michel Dupuis has extensive experience in research in theoretical and computational chemistry. He is the Associate Division Director of the Catalysis Science Department of the Chemical and Materials Sciences Division at the Pacific Northwest National Laboratory. Before joining PNNL in 1995, Dr. Dupuis was a Senior Scientist at IBM-Kingston, New York. He is the main author of the widely used HONDO program and a founding author of the GAMESS program for quantum chemical simulations.