

Carnegie Mellon University

Materials Science & Engineering

presents

Structure-Property Relationships in Nanostructured Materials: Aqueous Semiconductor Interfaces

Dr. Mark S. Hybertsen
Center for Functional Nanomaterials
Brookhaven National Laboratory

ABSTRACT:

Understanding structure-property relationships in fields as diverse as nanoscale electronic junctions, heterogeneous catalysis, electrochemistry and energy storage often starts by meeting the challenge of identifying key structure motifs. For the theorist this is followed by tackling the problem of calculating the relevant functional characteristics, also challenging, particularly for excited state properties. I will discuss the modern toolbox for these problems, including a brief outline of the basic physical ingredients of modern many-body perturbation theory which enables studies of excited state properties. I will then discuss its application in the context of the search to develop new materials for use in photocatalysis. In particular, I will discuss the search for key structural motifs at semiconductor-water interfaces and the connection to electrochemical energy level alignment.

Work performed in the Center for Functional Nanomaterials which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

BIOGRAPHY:

Mark S. Hybertsen holds a BA in Physics from Reed College in Portland, OR (1980) and a PhD in Physics from The University of California, Berkeley (1986) where his thesis research was directed to many-body perturbation theory and the GW approach. Dr. Hybertsen joined Bell Laboratories in 1986, pursuing a variety of research projects in the theory of the electronic properties of materials (bulk semiconductors, semiconductor surfaces and interfaces, cuprates, porous silicon, optoelectronic device physics). He supervised the Device and Materials Physics Group in the Semiconductor Photonics Research Department for four years. From 2003 to 2006, Dr. Hybertsen was a Senior Research Scientist in the Department of Applied Physics and Applied Mathematics at Columbia University in New York, where he has also been an Adjunct Professor in the Department of Electrical Engineering. In 2006, Dr. Hybertsen joined the new Center for Functional Nanomaterials at Brookhaven National Laboratory. He is a Senior Scientist, leading the Theory and Computation Group. He also maintains an adjunct research appointment at Columbia University. Dr. Hybertsen is a fellow of the American Physical Society and a member of the IEEE and the American Chemical Society.

Doherty Hall 2210, 11:30AM
Friday, December 8, 2017