Materials Science & Engineering Seminar Series

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Large Scale Simulations of Solid-liquid Interfaces Under Realistic Electrochemical Conditions for Energy Conversion and Storage

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ABSTRACT:

Solid-liquid interfaces are at the heart of a wide array of electrochemical technologies such as batteries, supercapacitors, fuel cells, electroactuators, and dye-sensitized solar cells. To optimize these technologies, the interactions of the charged electrodes and the ions from the surrounding electrolyte need to be understood at the molecular level. While existing quantum-mechanical models are applicable to either the electrolyte or the electrode in isolation, their combination is challenging using available computational approaches. This presentation will highlight progress in the quantum-continuum modeling of solid-liquid interfaces. The focus will be on the storage of energy in electrochemical capacitors and the production of chemical fuels in photoelectrochemical reactors. We will describe the use of newly developed, embedded quantum-mechanical techniques and large-scale finite-temperature sampling methods to elucidate pseudocapacitive storage at ruthenia electrodes and to predict the electrification of silicon photoelectrodes in realistic aqueous media.

BIOGRAPHY:

Ismaila Dabo graduated with a Ph.D. in Materials Science and Engineering from the Massachusetts Institute of Technology (MIT) in 2008. His doctoral research under the supervision of Dr. Marzari was dedicated to predicting the electrical response of quantum systems embedded in electrochemical environments and to studying chemical poisoning in low-temperature fuel cells. After graduation, Ismaila Dabo became a postdoctoral researcher and then a permanent researcher at Ecole des Ponts, University of Paris-Est (France). He joined the Department of Materials Science and Engineering at Penn State in 2013. He is a recipient of the ORAU Ralph E. Powe Junior Faculty Award and of the NSF Faculty Early Career Award (CAREER).

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