Designing Functional Materials with Engineered Defects One Atom at a Time

Date : Tuesday, October 2, 2018

Time : 1:00 pm – 2:00pm

Location : Engineering A-131

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Abstract:

Advances in first-principles calculations based on density-functional theory now make it possible to successfully describe the atomic-scale properties of "real" materials with defects and imperfections. Concurrent advances in scanning transmission electron microscopy enable imaging and spectroscopy of the atomic and electronic structure of materials with unprecedented spatial and energy resolution. This combination of theory and microscopy provides an unparalleled probe to unravel the structure-property correlations in real materials. These correlations when combined with advances in supercomputing and materials informatics — that enable high-throughput screening from thousands of often yet-to-be synthesized compounds — allow rational design of new materials with functionalities targeted for specific applications. New functional materials with engineered defects and imperfections are discussed for various energy applications, including design of lead-halide perovskites with defects engineered to achieve stable optoelectronic properties, lead-free perovskite semiconductors for use in solar cells, defective oxides for cleaner combustion of hydrocarbons, and inexpensive and durable catalysts for automotive fuel cells.

Bio:

Dr. Mishra received a Bachelor of Technology in Metallurgical and Materials Engineering from National Institute of Technology Karnataka in India (2008), and a PhD. in Materials Science and Engineering from The Ohio State University (2012). From 2012-2015, he was a postdoctoral researcher in the Scanning Transmission Electron Microscopy group at Oak Ridge National Laboratory, with a joint-affiliation from the Department of Physics and Astronomy at Vanderbilt University. He leads the Materials Modeling and Microscopy group (mcube.wustl.edu), with research interests in the rational design of materials for energy-related applications through a synergistic combination of electronic structure calculations and scanning transmission electron microscopy experiments.