Materials Science & Engineering Seminar Series

Carnegie Mellon University
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presents

Materials for Solar Energy Capture and Conversion by Scalable All-Electron First-Principles Simulations

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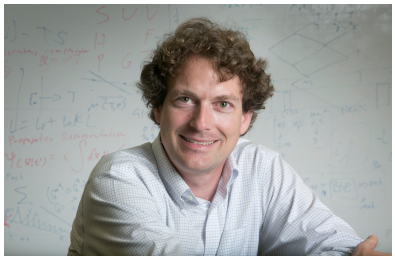
ABSTRACT: First-principles computational approaches are making steady progress to quantitatively predict, for specific materials, the conceptual phenomena that are central to phase stability, energy capture, energy conversion, and transport. This talk outlines the vision behind and ongoing evolution of an efficient, accurate all-electron computational framework for such simulations, FHI-aims [1], begun from scratch over ten years ago and now a global development by a large group of scientists and engineers spread around the globe. The primary methods are density-functional theory for ground-state properties and many-body approaches to capture excited-state phenomena. We highlight ongoing developments that extend our reach for hybrid density functional theory and the *GW* approach for charged excitations. The talk will then focus on understanding and predicting, in close collaboration with experimental colleagues, new energy conversion materials including carbon-nitrogen based materials for photochemical hydrogen evolution and new multinary materials for photovoltaics. Finally, we show how these approaches aid the discovery of new hybrid organic-inorganic materials incorporating complex organic molecules for energy and electronic applications.

[1] V. Blum *et al.*, Computer Physics Communications **180**, 2175 (2009);
http://aims.rz-berlin.mpg.de



BIOGRAPHY: Volker Blum is an Associate Professor in the Department of Mechanical Engineering and Materials Science at Duke University, Durham, NC. He obtained his doctoral degree from University of Erlangen, Germany, in 2001 and then pursued his post-doctoral research at National Renewable Energy Laboratory in Golden, CO, from 2002-2004. Prior to joining Duke University in 2013, he was a scientist and group leader at the Fritz Haber Institute in Berlin, Germany (2004-2013). He is an expert in first-principles based simulations of materials, molecules, and their properties and is the founding and lead developer of the globally developed all-electron electronic structure simulations package FHI-aims, used by over 100 groups in academia and industry. His current research focuses on computational predictions and understanding of new materials related to energy and electronics, as well as molecular structure and spectroscopies.

Doherty Hall 2210, 11:30AM
Friday, November 4, 2016