

Argonne Leadership Computing Facility Seminar

Speaker: Volker Blum, Duke University

Host: Alvaro Vazquez Mayagoitia

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Scalable, Efficient All-Electron First-Principles Simulation Approaches to Materials, Molecules, and Large Nanostructures

Computational simulations based on the first principles of quantum mechanics are now virtually indispensable as independent, non-empirical complements to analytical theory and experimental approaches across molecular and materials science. This talk describes the current and future directions of an efficient, accurate all-electron computational framework for such simulations, FHI-aims [1], begun from scratch over ten years ago and now developed by a large group of scientists and engineers spread around the globe. The primary methods are density-functional theory (DFT) for ground-state properties and many-body approaches to capture excited-state phenomena. The key algorithmic choice is the use of numeric atom-centered basis functions to discretize the orbitals and wave functions, enabling simulations of non-periodic (molecular) and periodic systems (solids, surfaces, nanostructures) from fast qualitative up to benchmark-quality numerical accuracy within one consistent framework. The code is proven up to several thousand atoms for DFT-based simulations and is scalable on current massively parallel high-performance computing platforms including Intel's KNL and NVidia's GPUs. A new, open-source infrastructure "ELSI" connects FHI-aims to even larger-scale simulations, incorporating several approaches to accelerate or circumvent the $O(N^3)$ eigenvalue solver scaling bottleneck of Kohn-Sham DFT in a library infrastructure that reaches beyond a single code. A particular focus of this talk will be phenomena in energy-related materials, including phase stability of predicted and new materials, electronic levels, and energy conversion. We highlight ongoing developments that extend our reach for hybrid density functional theory and the GW approach for charged excitations. Finally, we show how these approaches aid the discovery of new materials, for the particular example of new hybrid organic-inorganic materials incorporating functional organic molecules for light emission.

[1] V. Blum et al., *Computer Physics Communications* 180, 2175 (2009);

<http://aims.rz-berlin.mpg.de>

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. From 2004-2013, he was a scientist and group leader at the Fritz Haber Institute in Berlin, Germany. His current research focuses on computational predictions and understanding of new materials related to energy and electronics, as well as molecular structure and spectroscopies. Much of this work is directly connected to ongoing developments of new algorithms and computational tools in the all-electron electronic structure package FHI-aims and in the broader "ELSI" infrastructure.