DEPARTMENT OF PHYSICS & ASTRONOMY

CONDENSED MATTER SEMINAR

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Materials Physics from Simple to Complex Tunable Semiconductors from a Frist Principles Computational Approach

This talk summarizes ongoing work in our group to computationally capture materials properties, particularly of tunable new semiconductor materials for energy and electronics, using first principles simulations. Specific examples include (i) tunable hybrid organic-inorganic perovskite (HOIP) semiconductor incorporating functional organic molecules [1] and (ii) new multinary, defect-resistant chalcogenide-based semiconductor materials for photovoltaic and/or photovoltaic applications [2,3]. Both classes of materials can be synthesized as high-quality, precisely controlled crystals. However, their chemical structure is complex, challenging the reach of computational approaches to predict their atomic and electronic structure accurately prior to synthesis and/or in order to understand observed properties once a material has been made. Our primary computational tool for this is the FHI-aims [4] code, aided by a collaboratively developed, open-source infrastructure "ELSI" [5]. We outline our computational approach to capture electronic properties of complex semiconductors, using hybrid density functional theory including spin-orbit coupling, and highlight key examples of tailoring electronic levels and their alignment in new HOIP and chalcogenide semiconductors.

The methodological work reported in this talk would not be possible without the continued support and contributions from the very large community of developers and users of the FHI-aims code. Similarly, our work on materials predictions is critically influenced by close collaborations with leading experimental colleagues, particularly the group of David Mitzi (Duke University).

[1] C. Liu *et al.*, Physical Review Letters **121**, 146401 (2018); [2] T. Zhu *et al.*, Chemistry of Materials **29**, 7868-7879 (2017); [3] G.C. Wessler *et al.*, Chemistry of Materials **30**, 6566 (2018); [4] V. Blum *et al.*, Computer Physics Communications **180**, 2175 (2009); [5] V. W.-z. Yu *et al.*, Computer Physics Communications **222**, 267 (2018).

Tuesday, October 15, 2019

4:00 pm, JFB 334

Refreshments will be served in JFB 334 at 3:45 pm