All-electron theory of new inorganic and organic-inorganic semiconductors

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This talk describes some recent progress in our group regarding accurate, efficient all-electron approaches in computational simulations of new inorganic and organic-inorganic materials. We first cover recent progress in the FHI-aims all-electron code and in the open-source infrastructure "ELSI" for efficient, parallel simulations of materials with large system sizes using current, massively parallel supercomputing resources. Specific applications covered include joint experiment-theory work on the discovery of new defect resistant multinary chalcogenide semiconductors I2-II-IV-IV4 (e.g., Cu2BaSn(S,Se)4), as well as tunable organic-inorganic hybrid perovskite semiconductors including large, optically active organic components.

This overview talk covers joint work with many colleagues, including the groups of David Mitzi (Duke), Yosuke Kanai (UNC), Matthias Scheffler (FHI Berlin), Xinguo Ren (USTC Hefei), group members at Duke University, and the very large developer community of the FHI-aims code. Part of this work was supported by the National Science Foundation (CBET-1511737, DMR-1729297) and the US Department of Energy (CHOISE EFRC).