Benchmarking Electronic Structure Beyond Structural Properties of Solids

William P. Huhn[1] and V. Blum[1]

[1] Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC 27708, USA

The "Delta" benchmark between different electronic structure codes (https://molmod.ugent.be/deltacodesdft) served as a milestone for code verification in the computational materials science community, offering a comprehensive means to assess the relative precision of different implementations for basic structural properties of solids, across the periodic table. However, practical use cases demand a host of other observables, either in individual simulations or in high-throughput scenarios, and comprehensive sets of benchmarks are often unavailable in such cases. Energy band structures are such a case, complicated by the fact that different energy ranges must be captured and that a wide variety of different approaches to relativistic band-structure corrections exists in the literature. We conducted and provide a systematic set of band structure benchmarks [1] for 103 compounds including elements up to Bi (Z=83). The benchmark set covers scalar-relativistic case (DFT-PBE), where in principle all implementations should agree closely, as well as for different levels of spin-orbit coupling and for hybrid density functionals (HSE06). We use the all-electron codes FHI-aims and Wien2k as high-precision reference approaches. Within the FHI-aims code, a number of higher-level approaches to electronic structure are also available, lending themselves to future benchmark efforts both for molecules and solids; we comment particularly on benchmarking potential for GW and the Bethe-Salpeter Equation for neutral excitations.

References

[1] W. P. Huhn and V. Blum, Phys. Rev. Materials **1**, 033803 (2017).