Abstract Submitted
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Kohn-Sham Band Structure Benchmark Including Spin-Orbit Coupling for 2D and 3D Solids[1] WILLIAM HUHN, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA, VOLKER BLUM, Department of Mechanical Engineering and Material Science, Duke University, Durham, NC, USA — Accurate electronic band structures serve as a primary indicator of the suitability of a material for a given application, e.g., as electronic or catalytic materials. Computed band structures, however, are subject to a host of approximations, some of which are more obvious (e.g., the treatment of the exchange-correlation of self-energy) and others less obvious (e.g., the treatment of core, semicore, or valence electrons, handling of relativistic effects, or the accuracy of the underlying basis set used). We here provide a set of accurate Kohn-Sham band structure benchmarks, using the numeric atom-centered all-electron electronic structure code FHI-aims combined with the "traditional" PBE functional and the hybrid HSE functional, to calculate core, valence, and low-lying conduction bands of a set of 2D and 3D materials. Benchmarks are provided with and without effects of spin-orbit coupling, using quasi-degenerate perturbation theory to predict spin-orbit splittings.

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