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Benchmarking Post-SCF Treatments of Spin-Orbit Coupling in Electronic Structure Theory WILLIAM PAUL HUHN, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — Spin-orbit coupling (SOC) is an essential aspect of the electron band structures for all but the lightest-element materials. SOC is often incorporated into density-functional theory (DFT) calculations in a second-order variational approach, applying the SOC correction based on the orbitals from a scalar-relativistic self-consistent calculation. This talk compares the quality of non-self-consistent and self-consistent SOC corrections for a test set of over 100 different materials spanning the periodic table. We quantitatively compare entire DFT band structures from two benchmark-quality full-potential all-electron codes, i.e., the numeric atom-centered orbital code FHI-aims and the linearized augmented plane-wave code WIEN2k, based on the semilocal PBE functional. Few-meV agreement between non-self-consistent and self-consistent SOC is shown for elements up to row 4 of the periodic table, with agreement on the order of 10 meV for row 5 elements and differences exceeding 100 meV emerging for row 6 elements. We find little difference in SOC splittings between the PBE functional and the hybrid HSE06 functional.

William Paul Huhn
MEMS Department, Duke University, Durham, NC 27708

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