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Spin-Orbit Coupling within the GW Approximation[1] BRAD BARKER, University of California-Berkeley, Lawrence Berkeley National Laboratory, JACK DESLIPPE, National Energy Research Scientific Computing Center, MANISH JAIN, JOHANNES LISCHNER, University of California-Berkeley, Lawrence Berkeley National Laboratory, OLEG YAZYEV, Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland, STEVEN G. LOUIE, University of California-Berkeley, Lawrence Berkeley National Laboratory — We have developed and implemented an approach in which the effects of spin-orbit interactions to the quasiparticle band structure are incorporated within the GW approach, employing spinor wavefunctions computed at the density functional theory (DFT) level with fully relativistic pseudopotentials. Special consideration is given to the significance of the spin-dependent exchange-correlation potential. We compare these results to separate calculations where spin-orbit coupling is applied as a perturbation. We apply these methods to the properties of materials with heavy ion cores to determine the possible differences from the different treatments of spin-orbit coupling.

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