

Abstract Submitted
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A GW-based many-body perturbation theory approach for investigating materials with strong spin-orbit coupling BRADFORD BARKER, JACK DESLIPPE, OLEG YAZYEV, STEVEN LOUIE — Spin-orbit coupling is an essential ingredient in understanding the electronic properties of materials of recent interest. We have developed a means of incorporating spin-orbit coupling to the quasiparticle excitations in solids within the GW approach. We apply our method to the properties of materials with heavy ion cores. This work was supported by National Science Foundation Grant No. DMR10-1006184, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC.

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