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Spin-orbit coupling effects in excited-state phenomena: ab initio plane-wave-based GW and GW-BSE studies<sup>1</sup> MENG WU, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — The ab initio GW and GW-BSE methods based on many-body perturbation theory play an important role in understanding and predicting the electronic and optical properties of materials. And spin-orbit interaction introduces interesting spin physics and relativistic effects in materials such as III-V semiconductors and transition metal dichalcogenides that contain heavy elements. With full-spinor support in a plane-wave-based GW-BSE method, we study the effects of spin-orbit coupling in the quasiparticle and excitonic properties of several materials of current interest, including reduced dimensional systems.

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