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A Plane-Wave Implementation of Quasiparticle Self-Consistent GW (QSGW)[1] DEREK VIGIL CURREY, JACK DESLIPPE, STEVEN G. LOUIE, University of California-Berkeley and Lawrence Berkeley National Lab — The use of GW techniques in calculating the quasiparticle properties of certain classes of materials, e.g. complex oxides, is sometimes hindered by the poor mean-field starting point that density functional theory (DFT) within standard Kohn-Sham implementations provides. There has been considerable effort in the community to improve upon the mean-field starting point for a broad range of materials. A recently proposed method, the quasiparticle self-consistent GW (QSGW) method, employs a process in which a mean-field exchange-correlation potential is approximated from and updated self-consistently using the self-energy operator from previous iteration GW calculations. We present an implementation of this method in a plane-wave basis, and discuss its accuracy, computational cost, and physical implications for a variety of semiconducting materials.

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