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All-Electron *GW* Approximation in the Augmented-Plane-Wave Basis-Set Limit[1] CHRISTOPH FRIEDRICH, ARNO SCHINDLMAYR, STEFAN BLÜGEL, Forschungszentrum Jülich, Germany, TAKAO KOTANI, Arizona State University, Tempe, USA — The *GW* approximation for the electronic self-energy is known to yield quasiparticle band structures in very good agreement with experiment, but almost all codes so far rely on the pseudopotential approach, which restricts the range of materials that can be treated efficiently. In addition, the adequacy of the pseudopotential approximation for quasiparticle calculations has recently come under debate. We have developed an alternative implementation within the full-potential linearized augmented-plane-wave (FLAPW) method. As possible errors resulting from the linearization of the basis set are frequently overlooked, we here investigate the influence on the *GW* self-energy correction. A systematic improvement is achieved by including additional local orbitals defined as second and higher energy derivatives of solutions to the radial scalar-relativistic Dirac equation, which constitute a natural extension of the FLAPW basis set. Within this approach we can systematically reduce the linearization error and reach the exact augmented-plane-wave basis-set limit. While the electronic self-energy and the quasiparticle energies benefit from the better description of the unoccupied states, the resulting band gaps remain relatively unaffected.

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