GW method Based on the Full-Potential LMTO Method

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We present a new all-electron, augmented-wave implementation of the GW method. The eigenfunctions generating G and W are obtained using a recent variant of the full-potential LMTO method. The dynamical screening is fully taken into account without plasmon-pole models. The dynamically screened Coulomb interaction W is expanded in a mixed basis set which consists of two contributions, local atom-centered functions confined to muffin-tin spheres, and plane waves with the overlap to the local functions projected out. The local functions are calculated from products of solutions to the Schrodinger equation within the muffin-tin sphere, and can include any of the core states. Thus, the core functions may be treated on an equal footing with the valence electrons.

The model-free computation of screening together with the mixed basis make it feasible to investigate materials with rather localized electrons. We have applied this new method to some semiconductors, insulators, and metals. We will presents results for Si, Ge, C, GaN, GaAs, MgO, CaO, CdTe, HgTe, Ag, and CaB_6 with special attention to the difference the results of this method and other implementations of GW theory, and the contribution of the core and the core-like d