

Application of quasiparticle self-consistent GW to magnetic and metallic materials

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The GW approximation is well established as a method for predicting band gaps, effective masses, and optical properties of semiconductors and insulators with high accuracy and without empirical parameters [1,2]. In contrast, its applications to metals and magnetic materials remain limited, and no consensus has yet been reached on how GW corrections modify their electronic structure. For such systems, self-consistency is essential: the self-energy can shift bands across the Fermi level and thereby change the occupations, and hence the Fermi surface, the d-orbital occupations, and the spin moments. These changes must be fed back into the one-particle potential, which is not possible in the one-shot G_0W_0 approach based on LDA/GGA eigenstates. The quasiparticle self-consistent GW (QS GW) approach [1,2] constructs a static, Hermitian exchange-correlation potential from the self-energy $\Sigma = iGW$, with W evaluated in the random phase approximation, and iterates until G and W are consistent with the resulting quasiparticle states, including their occupations. QS GW thus provides a parameter-free description of metals and magnets that is independent of the starting point.

Here we present applications of QS GW to two metallic systems. For the magnetic shape memory alloy Ni_2MnGa , whose magnetic field-induced strain is associated with modulated martensite phases such as 10M and 14M, QS GW for the austenite phase yields a Lindhard-type susceptibility with a peak at the nesting vector corresponding to the 10M structure, predicting a 10M instability [3]. In the 10M and 14M phases, the Fermi level lies at the minimum of a valley in the Ni minority-spin density of states, suggesting electronic stabilization [4]; this feature is absent in GGA, which predicts the 10M phase to be metastable [5].

For the transparent superconductor LiTi_2O_4 , QS GW yields a narrower Ti 3d bandwidth and an enhanced density of states at the Fermi level compared with GGA, reflecting electron localization effects [6]. The QS GW dielectric function reveals pseudo-plasmons arising from interband transitions in the infrared region, which explain the optical transparency of this metallic oxide [6]. Furthermore, by combining QS GW with the cumulant expansion [7], we predict a plasmonic-polaron satellite, originating from a low-energy plasmon of the Ti 3d electrons at the Fermi level, which appears as a replica band in the valence band.

These results show that QS GW , through its self-consistent treatment, captures features of the electronic structure of metals and magnets beyond LDA/GGA. Comparisons with GGA and experiments will be discussed.

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