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QuasiParticle Self-Consistent, GW Theory TAKAO KOTANI, Osaka University, MARK VAN SCHILFGAARDE, Arizona State University, SERGEY FALIEEV, Sandia National Labs — A formal justification for a new kind self-consistent $GW$ approximation is developed. In this Landau-Silin picture the $GW$ approximation is based on the ansatz of the existence of bare quasiparticles generated from a noninteracting Hamiltonian $H_0$ and corresponding Green’s function $G_0$. In this picture, electrons and holes should have real meaning; $W$ is computed from the time-dependent Hartree approximation; $\Sigma = iG_0W$ means “exchange effect” + electrons and holes interacting. A key issue is how to construct the optimum $H_0$. The true Green’s function $G$ should have corresponding one-particle excitations, and $H_0$ should approximate the corresponding energies and eigenfunctions as well as possible. We present a prescription for $H_0$ that approximately minimizes the difference between $G^{-1}$ and $G_0^{-1}$. The theory is applied to $sp$ bonded materials, simple and transition metals, transition-metal oxides, some magnetic compounds such as MnAs and some $f$ systems (e.g. CeO$_2$, and Gd). We compare to a variety of experimental data for these different materials classes. The errors are quite small and highly systematic in $sp$ systems, they are somewhat larger but still systematic in transition-metal oxides, and are largest for Gd. Some analysis of the origin of the errors will be presented.

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