Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

QuasiParticle Self-Consistent, *GW* Theory TAKAO KOTANI, Osaka University, MARK VAN SCHILFGAARDE, Arizona State University, SERGEY FALEEV, 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.

Mark van Schilfgaarde
Arizona State University

Date submitted: 01 Dec 2004 Electronic form version 1.4