Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Self-consistent GW calculations with basis of dominant products
PETER KOVAL, Centro de Fisica de Materiales, DIETRICH FOERSTER, University of Bordeaux 1, DANIEL SANCHEZ PORTAL, Centro de Fisica de Materiales — Hedin's *GW* approximation (GWA) is a well known method to study charged excitations in electronic systems with a moderate computational cost [1]. Already one-shot GWA delivers a considerable improvement if compared with Green's functions from density-functional theory (DFT). However, the one-shot results are dependent on the used starting point. This unphysical dependence can be eliminated by iterating a *GW* calculation to self-consistency. We implemented self-consistent GWA for molecules [2], within our original framework of dominant products basis. We use the DFT calculation by SIESTA code as starting point. The framework allowed to calculate Green's functions on a fine frequency mesh for such small molecules as benzene. We demonstrate the level of independence on starting point achievable within pseudo-potential framework, validating the implementation. Effects of the self-consistency on the interacting Green's function will be discussed along with different levels of self-consistency and mixing schemes. Finally, we compare the self-consistency with so-called quasi-particle self-consistent *GW* [3].

[1] F.Aryasetiawan, O.Gunnarsson, Rep. Prog. Phys. 61, 237 (1998).
[2] D.Foerster, P.Koval, D.Sanchez Portal, J. Chem. Phys. 135, 074105 (2011).
[3] T.Kotani, M.van Schilfgaarde, S.V.Falleev, Phys. Rev. B 76, 165106 (2007).

Peter Koval
Centro de Fisica de Materiales

Date submitted: 29 Nov 2011 Electronic form version 1.4