Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Unified description of ground and excited states of finite systems: the self-consistent *GW* approach FABIO CARUSO, PATRICK RINKE, XINGUO REN, Fritz Haber Institute, Berlin, Germany, ANGEL RUBIO, Universidad del Pais Vasco, San Sebastian, Spain, MATTHIAS SCHEFFLER, Fritz Haber Institute, Berlin, Germany — Fully self-consistent *GW* calculations – based on the iterative solution of the Dyson equation – provide an approach for consistently describing ground and excited states on the same quantum mechanical level. Based on our implementation in the all-electron localized basis code FHI-aims [1], we show that for finite systems self-consistent *GW* reaches the same final Green function regardless of the starting point. The results show that self-consistency systematically improves ionization energies and total energies of closed shell systems compared to perturbative *GW* calculations (G_0W_0) based on Hartree-Fock or (semi)local density-functional theory. These improvements also translate to the electron density as demonstrated by a better description of the dipole moments of hetero-atomic dimers and the similarity with the coupled cluster singles doubles (CCSD) density. The starting-point independence of the self-consistent Green function facilitates a systematic and unbiased assessment of the performance of the *GW* approximation for finite systems. It therefore constitutes an unambiguous reference for the future development of vertex corrections and beyond *GW* schemes. [1] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

Fabio Caruso
Fritz Haber Institute, Berlin

Date submitted: 11 Nov 2011 Electronic form version 1.4