Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Many-body perturbation theory using the density-functional concept: beyond the GW approximation FABIEN BRUNEVAL, Ecole Polytechnique, CEA, CNRS, FRANCESCO SOTTILE, VALERIO OLEVANO, RODOLFO DEL SOLE, LUCIA REINING, INFM, Universita di Roma Tor Vergata — Electronic structure calculations based on the Many-Body Perturbation Theory (MBPT), within GW approximation [1], are very reliable for simple materials. Some failures (e.g. for transition metals) ask for better approximations that could be in principle derived through the usual set of MBPT equations. This procedure would be however computationally prohibitive. We propose an alternative formulation of MBPT that relies on density-functional concept [2]. Our equation for the polarizability is a two-point one, that leads to excellent optical absorption and energy loss spectra [3]. The other MBPT quantities are then simply calculated via an integration. The terms beyond GW approximations, that we obtain, are both more simple and more physically intuitive, than the usual ones. We show a direct impact of this formulation on the TDDFT. Numerical results for optical absorption, IXS, and the band gap of bulk silicon and solid argon illustrate the leading corrections beyond RPA for the polarizability and GW for the self-energy. [1] L. Hedin, Phys. Rev. **139**, A796 (1965). [2] F. Bruneval *et al.*, submitted to Phys. Rev. Lett. [3] F. Sottile, V. Olevano, and L. Reining, Phys. Rev. Lett. **91**, 056402 (2004).

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Date submitted: 22 Mar 2013 Electronic form version 1.4