Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Beyond the *GW* approximation: a second-order screened exchange correction PATRICK RINKE, FABIO CARUSO, XINGUO REN, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, Berlin, Germany, NOA MAROM, University of Texas, Austin, USA — Despite the success of the *GW* method in describing the photoemission spectra of solids, molecules and clusters, challenges remain. For aromatic molecules for example absolute as well as relative positions of ionisation energies and affinities are not well reproduced in perturbative G_0W_0 schemes with different starting points as well as in self-consistent *GW* [1], sometimes even giving the wrong orbital order. Motivated by renormalized second-order perturbation theory [2] for the ground-state energy, we propose a second-order screened exchange correction (SOSEX) to the *GW* self-energy. This correction follows the spirit of the SOSEX correction to the random-phase approximation for the electron correlation energy and reduces the self-correlation error. The performance of the *GW*+SOSEX scheme has been benchmarked for a set of molecular systems, including the G2 set, commonly used acceptor molecules, benzene and the azabenzene molecules. We find that the SOSEX correction improves the description of the spectral properties including the orbital order with respect to the different *GW* schemes, highlighting the importance of reducing the self-correlation error.

[1] N. Marom *et al.*, arXiv:1211.0416
[2] X. Ren *et al.*, J. Mater. Sci. **47**, 7447 (2012)

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Date submitted: 07 Nov 2012 Electronic form version 1.4