Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Objective performance of the GW approximation and the Bethe-Salpeter Equation for molecules FABIEN BRUNEVAL, CEA, SRMP (France) & Dept. of Physics, UC Berkeley & Lawrence Berkeley National Lab (USA), SAMIA M. HAMED, TONATIUH RANGEL-GORDILLO, JEFFREY B. NEATON, Dept. of Physics, UC Berkeley & Lawrence Berkeley National Lab (USA) — We have evaluated the quality of the quasiparticle energies obtained within the *GW* approximation and of the optical excitations with the solution of the Bethe-Salpeter equation (BSE) for molecules. The calculations have been performed with a recently developed code based on Gaussian [1,2] that allowed us to use the exact same techniques as the one employed in traditional quantum chemistry. We demonstrate [3] the extreme sensitivity of the *GW* and BSE results upon the Kohn-Sham starting point. Most of the starting point dependence in BSE is to be ascribed to the underlying *GW* band structure. We highlight the problem of the triplet excitations that are equally underestimated in time-dependent density-functional theory and in BSE. [1] F. Bruneval, J. Chem. Phys. **136**, 194107 (2012). [2] F. Bruneval and M.A.L. Marques, J. Chem. Theory Comput. **9**, 324 (2013). [3] F. Bruneval, S. M. Hamed and J. B. Neaton, J. Chem. Phys. **142**, 244101 (2015).

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Date submitted: 02 Nov 2015 Electronic form version 1.4