Abstract Submitted
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Large Scale Many-Body Perturbation Theory calculations: methodological developments, data collections, validation[1] MARCO GOVONI, GIULIA GALLI, Argonne National Laboratory and University of Chicago — Green's function based many-body perturbation theory (MBPT) methods are well established approaches to compute quasiparticle energies and electronic lifetimes. However, their application to large systems – for instance to heterogeneous systems, nanostructured, disordered, and defective materials – has been hindered by high computational costs. We will discuss recent MBPT methodological developments leading to an efficient formulation of electron-electron and electron-phonon interactions, and that can be applied to systems with thousands of electrons. Results using a formulation that does not require the explicit calculation of virtual states, nor the storage and inversion of large dielectric matrices will be presented. We will discuss data collections obtained using the WEST code [1], the advantages of the algorithms used in WEST over standard techniques, and the parallel performance. Work done in collaboration with I. Hamada, R. McAvoy, P. Scherpelz, and H. Zheng.

[1] M. Govoni, and G. Galli, "Large scale GW calculations", J. Chem. Theory Comput. 11, 2680 (2015); www.west-code.org.

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