Abstract Submitted
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Efficient G_0W_0 using localized basis sets: a benchmark for molecules[1] PETR KOVAL, MATHIAS PER LJUNGBERG, Donostia International Physics Center, DANIEL SANCHEZ-PORTAL, Centro de Fisica de Materiales — Electronic structure calculations within Hedin's GW approximation are becoming increasingly accessible to the community. In particular, as it has been shown earlier and we confirm by calculations using our **MBPT_LCAO** package, the computational cost of the so-called G_0W_0 can be made comparable to the cost of a regular Hartree-Fock calculation. In this work, we study the performance of our new implementation of G_0W_0 to reproduce the ionization potentials of all 117 closed-shell molecules belonging to the G2/97 test set, using a pseudo-potential starting point provided by the popular density-functional package **SIESTA**. Moreover, the ionization potentials and electron affinities of a set of 24 acceptor molecules are compared to experiment and to reference all-electron calculations.

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