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Bridging the size gap between density-functional and many-body perturbation theory PAOLO UMARI, CNR-INFM Democritos — The calculation of quasi-particle spectra based on the GW approximation is extended to systems of hundreds of atoms and the calculation of empty states is avoided. This is achieved through an optimal strategy, based on the use of Wannier-like orbitals, for obtaining a basis for the polarization propagator. Then, a Lanczos chain approach permits to calculate the self-energy. Our method is validated by calculating the vertical ionization energies of the benzene molecule and the band structure of crystalline silicon. Its potentials are then demonstrated by addressing the quasi-particle spectrum of models of vitreous materials, as well as of large organic molecules.

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