

Electron-hole excitations in the quasiparticle picture and in the density-functional framework

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Ab initio calculations based on density functional theory (DFT) are a powerful tool for the study of ground state properties of even complex systems. In the case of electronic spectra, however, approaches have to be designed that extend existing methods to the description of electronic excitations. Today, two main lines of research seem to compete for the calculation of electron-hole excitations (that occur, e.g. in absorption or electron-energy loss spectroscopy): first, the GW and Bethe-Salpeter approaches, derived in the framework of many-body Green's function theory [1] generally yield spectra in good agreement with experiment, although with a considerable computational effort. Second, time-dependent density functional theory (TDDFT) [2] could in principle be more efficient, but suffers from the lack of reliable approximations for the exchange-correlation contributions; therefore, in particular absorption spectra of bulk materials are in general not well described.

We will compare the two approaches [3] by investigating the meaning and importance of their various ingredients, by pointing out similarities and differences in the formalisms, and by showing results for various materials ranging from nanotubes to bulk semiconductors and insulators. Finally, we conclude that the two approaches are not in competition, but that their advantages should be combined [4] in order to yield a reliable but efficient method for the calculation of electronic spectra of materials.

**with contributions from S. Botti, A. Marinopoulos, F. Sottile, V. Olevano, N. Vast, A. Rubio, G. Onida*

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