exciting NEWS

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The description of excitations in condensed matter poses serious challenges from a theoretical and computational viewpoint. A first fundamental example is the quasi-particle band structure of hybrid systems beyond the Kohn-Sham level of density-functional theory (DFT). Indeed, for hybrid materials, extension of the theory to include the *GW* methods is essential to describe physical and technological relevant properties like band gap alignments. A further example at a higher theoretical level is the formation of electron-hole pairs upon excitation by light, which are characterized by their binding strength, spatial extension and lifetime. This phenomenon, appearing, *e.g.*, in optical and x-ray absorption is quantitatively accounted for by the Bethe-Salpeter equation of many-body perturbation theory (MBPT). An alternative is time-dependent DFT, which is less well suited for strong excitonic effects in periodic systems.

In this talk I will present showcases of *ab-initio* calculation of excitations performed with the all-electron full-potential computer package **exciting**. This code is a full-potential all-electron DFT code, implementing the (linearized) augmented planewave + local-orbital [(L)APW+lo] method. This is known to be the gold standard for solving the Kohn-Sham equations of DFT. **exciting** provides as well sophisticated implementations of the concepts of MBPT, in particular, the *GW* approach for obtaining the quasi-particle band structure and the Bethe-Salpeter equation for treating optical and core-level spectra. I will provide a review of these methods, discussing benefits and challenges, and will introduce the latest developments and implementations like, for example, resonant inelastic x-ray scattering (RIXS)**.**