MAR16-2015-004815

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Quasiparticle energies, excitonic effects, and dielectric screening in transparent conducting oxides

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Using the power of high-performance super computers, computational materials scientists nowadays employ highly accurate quantum-mechanical approaches to reliably predict materials properties. In particular, many-body perturbation theory is an excellent framework for performing theoretical spectroscopy on novel materials including transparent conducting oxides, since this framework accurately describes quasiparticle and excitonic effects.

We recently used hybrid exchange-correlation functionals and an efficient implementation of the Bethe-Salpeter approach to investigate several important transparent conducting oxides. Despite their exceptional potential for applications in photovoltaics and optoelectronics their optical properties oftentimes remain poorly understood: Our calculations explain the optical spectrum of bixbyite indium oxide over a very large photon energy range, which allows us to discuss the importance of quasiparticle and excitonic effects at low photon energies around the absorption onset, but also for excitations up to 40 eV. We show that in this regime the energy dependence of the electronic self energy cannot be neglected. Furthermore, we investigated the influence of excitonic effects on optical absorption for lanthanum-aluminum oxide and hafnium oxide. Their complicated conduction band structures require an accurate description of quasiparticle energies and we find that for these strongly polar materials, a contribution of the lattice polarizability to dielectric screening needs to be taken into account. We discuss how this affects the electron-hole interaction and find a strong influence on excitonic effects.

The deep understanding of electronic excitations that can be obtained using these modern first-principles techniques, eventually will allow for computational materials design, e.g. of band gaps, densities of states, and optical properties of transparent conducting oxides and other materials with societally important applications.