Ab-initio calculation of electronic and optical properties of transparent conductive oxides

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Parameter-free calculations are a modern and sophisticated complement to advanced experimental techniques when exploring the properties of materials. Due to the rapidly increasing computing power they promise a deep understanding of the underlying physics also for more complex transparent conductive oxides.

We take the excitation aspect of photoemission processes into account by calculating the quasiparticle electronic structure using the modern HSE03+G_0W_0 framework. Solving a Bethe-Salpeter equation for the optical polarization function allows us to account for excitonic and local-field effects that govern the optical absorption.

After an introduction into these recent theoretical-spectroscopy techniques we apply them to ZnO, SnO_2, In_2O_3, and Ga_2O_3. We present results for the electronic band structure (including spin-orbit coupling), the band alignment, dielectric functions, exciton binding energies, and optical oscillator strengths. The influence of a degenerate electron gas, which occurs in these typically n-type materials, is investigated. Our findings are discussed with respect to available experimental results.

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