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Accurate surface ionization potentials and electron affinities of semiconductors and insulators, a step toward water splitting predictions[1]
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Design of semiconductors for water splitting requires knowledge of the position of band edges relative to the water redox potential. This can be achieved by predicting materials' ionization potentials (IPs) and electron affinities (EAs). We recently developed a predictive method combining different electronic structure techniques, which is able, as will be demonstrated, to reproduce IPs and EAs of a broad range of materials including standard semiconductors (GaAs, ZnO, CdS,...) and transition metal compounds (TiO2, MnO,...). Achieved accuracy is within 0.1-0.2 eV from the measured photoemission data. We use GGA(+U) to calculate the electronic structure of bulk systems and their surfaces leading to the alignment of the bulk GGA(+U) band edges with the vacuum. The many-body, quasiparticle GW method is used to calculate shifts of the bulk band edges with respect to the underlying GGA(+U) formalism. Combining GGA(+U) and GW results in accurate IPs and EAs. In the case of transition metal compounds additional external d-potentials are included in the selfconsistent GW cycle to account for the inaccurate position of the transition metal d-orbitals relative to s and p-orbitals, leading to accurate IPs and EAs also in these, for the electronic structure methods problematic, cases.

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