Modeling organohalide perovskites for photovoltaic applications: From materials to interfaces

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The field of hybrid/organic photovoltaics has been revolutionized by organohalide perovskites. A first-principles simulation toolbox is presented, along with the fundamental modeling strategies, using selected examples of relevant materials and interfaces. The main issue with hybrid perovskite modeling is to accurately describe their structural, electronic and optical features. These materials show a degree of short range disorder, due to the presence of mobile organic cations embedded within the inorganic matrix, requiring to average their properties over a molecular dynamics trajectory. Due to the presence of heavy atoms their electronic structure must take into account spin-orbit coupling (SOC) in an effective way, possibly including GW corrections.

Modeling charge generation in perovskite-sensitized TiO2 interfaces is then approached based on a SOC-DFT scheme, describing alignment of energy levels in a qualitatively correct fashion. The role of interfacial chemistry on the device performance is finally discussed.

References: