Semiconductor band alignment from first principles: a new nonequilibrium Green's function method applied to the CZTSe/CdS interface for photovoltaics - DTU Orbit (23/12/2018)

In this paper we present a method to obtain the band offset of semiconductor heterointerfaces from Density Functional Theory together with the nonequilibrium Green's function method. Band alignment and detailed properties of the interface between Cu₂ZnSnSe₄ and CdS are extracted directly from first principles simulations. The interface is important for photovoltaics applications where in particular the band offsets are important for efficiency. The band bending pose a problem for accurate atomistic simulations of band offsets due to its long range. Here we investigate two different methods for dealing with band bending directly. One involves doping the materials to induce a shorter screening length. The other method is to apply a voltage bias across the interface to correct for the band bending. The calculated band offsets agree well with previous experimental and theoretical studies and, interestingly, the offset is seen to depend on whether or not the interface is under flat-band conditions.