

Computational modeling of band gaps in perovskitesO. Syzgantseva¹, U. Röthlisberger^{1*}¹EPF Lausanne

Finding new semiconductor materials with specific band gaps, in particular within the class of perovskite compounds, is essential for the development of optoelectronic and photovoltaic applications. The screening of a wide compositional range of potentially suitable candidates requires elaboration of an accurate and fast computational methodology for the band gap evaluation. In this work, the band gaps in a series of doped perovskite materials are computed within the Density Functional theory. The impact of spin-orbit coupling, temperature and excitonic effects (BSE calculations) on the band gap value is analyzed as a function of dopant type and concentration. The applied methodology is iteratively assessed by dint of comparison with the experimental data for these systems. This approach is demonstrated to provide a close estimate of band gaps in doped perovskite compounds.