Computational modeling of band gaps in perovskites

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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.