Electronic properties of fluorides by efficient approximated quasiparticle DFT-1/2 and PSIC methods: CaF\(_2\), BaF\(_2\) and CdF\(_2\) as test cases

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Dialkali halides are materials of great interest from both fundamental and technological viewpoint, due to their wide transparency range. The accurate determination of their electronic, excitations and optical properties in bulk and low dimensional systems is therefore of crucial importance nowadays. Here we report electronic quasiparticle band structures for three representative bulk fluorides, CaF\(_2\), BaF\(_2\) and CdF\(_2\), calculated using two methods, the DFT-1/2 and the PSIC schemes, which have been relatively little explored by the theoretical community, so far. Our results, compared with both available experimental data and previous DFT-GW self-energy calculations, demonstrate a satisfying accuracy for the examined compounds, at a level comparable with the perturbative G\(_0\)W\(_0\) approach. Remarkably, both our proposed methods scale quite similarly to standard local density functional approaches, thus resulting in a large saving of computational effort with respect to the computationally heavyweight GW. Our results opens up the perspective of the computational exploration of much bigger fluoride systems. As a significant proof of concept of this capability, we also calculated by the DFT-1/2 approach the quasiparticle properties of the (111) surfaces of all the three systems under study.

References


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