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Electronic structure and charge transport properties in FASnI3-xBrx

The challenge of finding an earth-abundant non-toxic perovskite material suitable for solar cell applications brought about FASnX3, where the formamidium (FA) molecule replaces the (usually) large A cation and Sn bypasses the use of Pb, while keeping the electronic band gap in the range suitable for the visible spectrum light absorption.[1]

We investigate systematically the electronic structure of the FASnI3-xBrx compound series by means of first-principles calculations. On the basis of hybrid density functional theory and including spin-orbit coupling effects, we demonstrate the indirect influence that the formamidium molecule has on the electronic band gap. The prevalent and thus unavoidable nature of the electron-phonon coupling[2] justifies our investigation of the temperature-dependent polaron mobility. Here, we base our approach in the form of variational Feynman path integral applied to the Fröhlich-type polarons[3], i.e. long-range polarons. In this case, we extract the phonon parameters from a Gamma-point density functional perturbation theory calculation. We analyze the influence of both electron and hole polarons formation on the temperature dependence on the band gap.

[1] G. Nasti and A. Abate, Adv. Energy Mater. 2020, 10, 1902467

[2] Ghosh et al., J. Phys. Chem. Lett. 2020, 11, 3271-3286

[3] J.M. Froost, Phys. Rev. B 96, 195202 (2017)

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