Impact of electron-phonon scattering on optical and electrical properties of bulk semiconductor materials

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We present a numerical study of the impact of electron-phonon scattering (EPS) on the electronic density of states (DOS) of bulk semiconductor materials (GaAs and CH3NH3PbI3). In order to calculate the DOS in a perturbated system, we use a model based on Green functions formalism [1]. We achieved to determine the DOS decreasing behavior in the bandgap. This behavior depends on the strength of the EPS (Fig. 1.a), but also depends on the phonon energy. Electron-phonon interactions have a straightforward impact on material optical properties. Indeed, the presence of electronic states within the bandgap allows absorption and emission of photons with an energy lower than this material bandgap. As shown in Fig. 1.b, the emission spectrum can be widely disturbed by this interactions. For purposes of photovoltaic systems, in both GaAs and perovskite materials, we report a decrease in the absorption/emission ratio when the EPS strength increases, and therefore a efficiency reduction [2]. This degradation is all the more important as the carrier mobility is low.

[1] N.Cavassilas, F.Michelini, M.Bescond, « Modeling of Nanoscale Solar Cells : The Green's Fuction Formalism », J.Renewable Sustainable Energy 6, 011203 (2014)
[2] L.C.Hirst and N.J.Ekins-Daukes, Progress in Photovoltaics. Research and Applications 19,286 (2011)

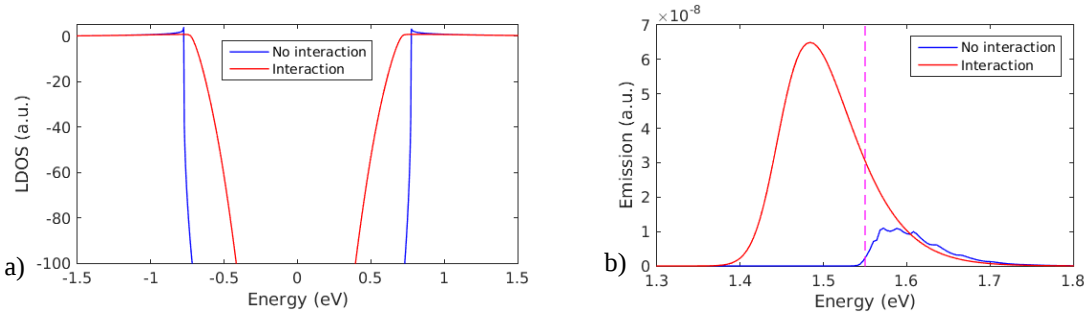

Figure 1 : a) Logarithm of the electronic density of states in CH3NH3PbI3 with and without electron-phonon scattering. b) Emission spectrum of CH3NH3PbI3 with and without interaction.