Impact of Electron-Phonon Scattering on Optical and Electrical Properties of Perovskite Material

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Perovskite materials are suitable for solar applications due to their excellent carrier transport properties [1,2]. However, behaviors controlling the carrier mobility, measured experimentally from 1 to 100 cm²/V.s [3,4], are not yet well understood. In this polar material it is generally assumed that interaction with polar optical phonon is important. However, rotations of the CH_3NH_3 matrix could also have an impact. From a formalism point of view, such rotations are very close to the polar phonon interaction, but with unknown parameters. In this work, we present a numerical study of electrical and optical properties modified by scattering. Using a non-equilibrium Green functions model [5] we obtain 196 cm²/V.s for the electron mobility. In order to fit the wide range of the experimental mobility we modify and assume four values of the coupling strength with the idea to mimic the CH_3NH_3 rotations. With this model we calculate the local density-of-states (DOS) in a perovskite-based device (Fig.1) which can be compared to the ballistic counterpart (Fig.2). Scattering tends to induce a broadening in the bandgap, that decrease exponentially in the latter. Fig. 3 and 4 respectively show the optical absorption and emission spectra for the four scattering couplings. Modifications with stronger scattering are both absorption and emission occurring at energies lower than the bandgap (1.55 eV). More important, we report Fig. 5 a decrease of the absorption/emission ratio inducing a reduction of the solar cell efficiency. We finally propose an analytical model of the DOS deep in the bandgap which is in good agreement with numerical results (Fig. 6).

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[3] Mei, Y et al., MRS Communications. 5. 1-5. 10.1557/mrc.2015.21 (2015).
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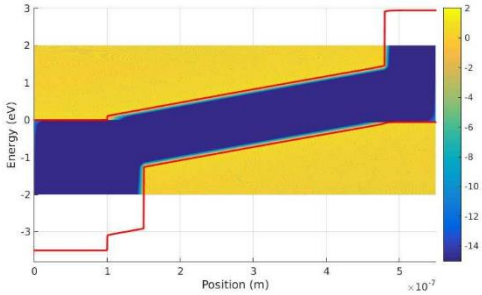

Fig.1: Log of local density of states as a function of energy and position in a perovskite-based solar cell, calculated without electron-phonon interaction.

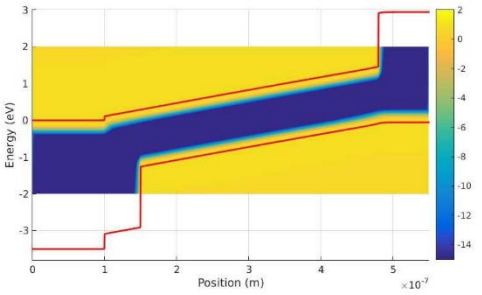

Fig.2: Log of local density of states as a function of energy and position in a perovskite-based solar cell, calculated with electron-phonon interaction (corresponding to a electron mobility = 86cm²/V.s)

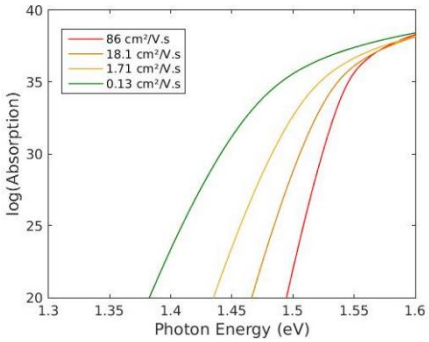

Fig.3: Log of absorption vs photon energy in the studied perovskite device, calculated for 4 different values of electron mobility (corresponding to 4 different values of electron-phonon scattering strength)

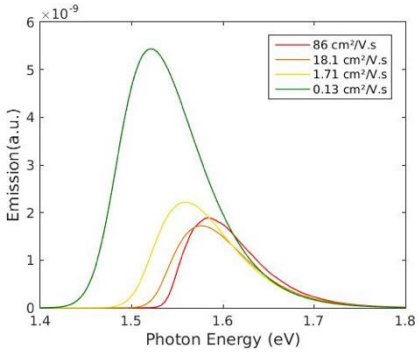

Fig.4 Emission vs photon energy in the studied perovskite device, calculated for 4 different values of electron mobility (corresponding to 4 different values of electron-phonon scattering strength)

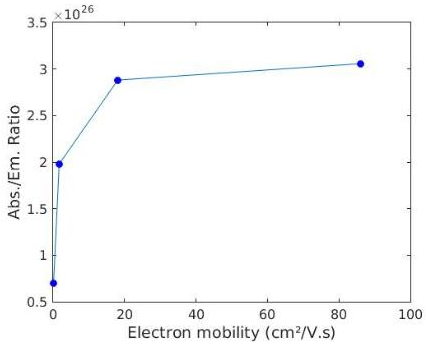

Fig.5: Absorption/emission ratio plotted as a function of electron mobility

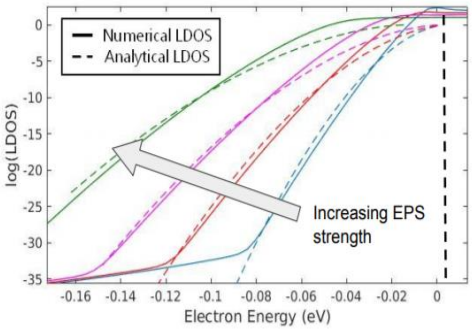

Fig.6: Log of local density of states close to the conduction band edge at the middle of the studied device. Plain lines correspond to self-consistent calculations. Dashed lines correspond to the analytical model.