Charge Carrier Dynamics in Lead Halide Perovskite Solar Cell: Effect of External Electric Field

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Lead halide perovskites have attracted much attention as an active material in solar cells.[1-3] In this first-principles study, we explore the optoelectrical properties of a solar cell composed of cesium lead halide perovskite thin film sandwiched between titanium dioxide cluster and organic dye. The titanium dioxide cluster serves as the electron transfer material which bonds to the perovskite surface through hydroxy groups, whereas the organic dye serves as the hole transfer material which bonds to the perovskite surface through methoxy groups. We apply external electric field normal to the surface of the perovskite thin film and find that there is a linear relationship between the band gap and the external electric field. The band gap decreases from 2.25 to 0.11 eV with the increase of external electric field from -0.30 to 0.05 eV/Å. Furthermore, we investigate the effect of external electric field onto charge carrier relaxations upon photoexcitation. The charge carrier dynamics providing rates of electron and hole relaxation and relaxation pathways, are calculated using reduced density matrix in the formalism of Redfield theory.[4-7] The relaxation rates of charge carriers depend on several factors such as energies of orbitals and spatial distributions of orbitals along the relaxation pathways.

References

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