Theoretical Study on Energy Conversion Processes of Perovskite Solar Cells

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Methylammonium (MA) lead iodide perovskite (CH3NH3PbI3) plays an important role in light absorption and carrier transport in efficient organic−inorganic perovskite solar cells [1]. Spin-polarized DFT calculations have been performed with the GGA. Effective masses of photogenerated electrons and holes are estimated to be 0.23m0 and 0.29m0, respectively, including spin−orbit coupling effects. This result is consistent with the long-range ambipolar transport property and with the large diffusion constants for both electrons and holes in the perovskite, which enable efficient photovoltaic conversion [2]. We also have focused our attention on the MA cation and studied the role it plays in the electronic/optical features of the perovskite [3]. An analysis of hot-carrier lifetimes from electron-phonon interaction in lead iodide perovskites using density-functional perturbation theory and many-body perturbation theory [4] shows that the holes in the perovskite have very long lifetimes in the valence band region situated 0.9eV below the top of the valence band. We propose a reduction of the relaxation paths in the small valence density of states as being the origin of the slow hot-hole cooling [5].

We have also characterized models of zero-dimensional (cluster) MAPbI3 perovskite systems [6,7]. Interesting properties of such clusters include their charge distribution, bandgap, wave function localization, and reduced effective mass. The aim of this study is to pave the way for further investigations of clusters with different orientations, terminations, and compositions.

References

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