[14p-1G-2] Photoinduced Carrier-Transfer Dynamics at Surfaces/Interfaces

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The effective masses of photocarriers and the role of methylammonium (MA) cation in CH$_3$NH$_3$PbI$_3$ are studied based on density functional theory. Effective masses of photogenerated electrons and holes are estimated to be $m_e^* = 0.23m_0$ and $m_h^* = 0.29m_0$, respectively, including spin–orbit coupling effects. This result is consistent with the long-range ambipolar transport property and with the larger diffusion constant for electrons compared with that for holes in the perovskite, which enable efficient photovoltaic conversion. We also have focused our attention on the MA cation and studied the role it plays in the electronic/optical features of the perovskite.