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Rashba Spin-Orbit Coupling Enhanced Carrier Lifetime in $CH_3NH_3PbI_3$[1] FAN ZHENG, LIANG Z. TAN, University of Pennsylvania, SHI LIU, Carnegie Institution for Science, ANDREW M. RAPPE, University of Pennsylvania — Organometal halide perovskites are promising solar-cell materials for next-generation photovoltaic applications, in particular these materials have long carrier lifetime and diffusion length. Recently, the strong spin-orbit coupling of organometal halide perovskites have attracted the great attention, the consequences of the Rashba effect, driven by this strong spin-orbit coupling, on the photovoltaic properties of these materials are largely unexplored. In this work, taking the electronic structure of methylammonium lead iodide as an example, we propose an intrinsic mechanism for enhanced carrier lifetime in 3D Rashba materials. Based on first-principles calculations and a Rashba spin-orbit model, we demonstrate that the recombination rate is reduced due to the spin-forbidden transition. These results are important for understanding the fundamental physics of organometal halide perovskites and for optimizing and designing the materials with better performance. The proposed mechanism including spin degrees of freedom offers a new paradigm of using 3D Rashba materials for photovoltaic applications.

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