

# Rashba Spin-Orbit Coupling Enhanced Carrier Lifetime in Organometal Halide Perovskites

Fan Zheng, Liang Z. Tan, Shi Liu, and Andrew M. Rappe  
The Makineni Theoretical Laboratories, Department of Chemistry, University of  
Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA

Organometal halide perovskites are promising solar-cell materials for next-generation photovoltaic applications. The long carrier lifetime and diffusion length of these materials make them very attractive for use in light absorbers and carrier transporters. Previous studies reported a relatively low defect concentration in  $\text{CH}_3\text{NH}_3\text{PbI}_3$ , which reduces the scattering centers for nonradiative charge carrier recombination. Recently, it has been suggested that the spatial carrier segregation caused by disorder-induced localization or domains acting as internal  $p$ - $n$  junctions may reduce the recombination rate. While these aspects of organometal halide perovskites have attracted a great deal of attention, the consequences of the Rashba effect [1], driven by 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.

[1] M. Kim, J. Im, A. J. Freeman, J. Ihm, and H. Jin, Proc. Natl. Acad. Sci. 111, 6900 (2014).