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First-principles investigation of charge carrier trapping at surface defects of organic-inorganic hybrid perovskites as photovoltaic materials[1]

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— Organic-inorganic hybrid perovskites (OIHPs) such as $CH_3NH_3PbI_3$ are attracting much interest for photovoltaic application. One of the determining factors of their performance is charge carrier trapping at defects on their surface or grain boundaries. For example, remarkable improvement of photoconversion efficiency from 13.1 % to 16.5 % was achieved by surface passivation with Lewis bases due to suppression of charge carrier trapping at surface defects[2]. However, the chemical nature of such surface defects (e.g. vacancy or interstitial) is still not well understood. In this work, types of surface defects responsible for charge carrier trapping were clarified by comprehensive first-principles investigation of various types of defects using slab models. It is shown that the defect states originated in Pb-Pb covalent bonding orbitals formed by excessive Pb atoms on OIHPs surface are responsible for charge carrier trapping. Our result paves the way for improvement of the photovoltaic performance of OIHPs through rational strategy of suppressing charge carrier trapping at surface defects.

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[2]N. K. Noel, A. Abate, S. D. Stranks, E. S. Parrott, V. M. Burlakov, A. Goriely, and H. J. Snaith, *ACS Nano* **8**, 9815 (2014)

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