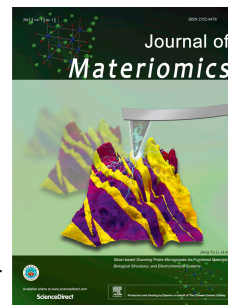


Accepted Manuscript

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PII: S2352-8478(15)00052-0

DOI: [10.1016/j.jmat.2015.07.005](https://doi.org/10.1016/j.jmat.2015.07.005)

Reference: JMAT 26

To appear in: *Journal of Materiomics*

Received Date: 21 May 2015

Revised Date: 9 July 2015

Accepted Date: 15 July 2015

Please cite this article as: Geng W, Tong C-J, Tang Z-K, Yam C, Zhang Y-N, Lau W-M, Liu L-M, The Effect of the Surface Composition on Electronic Properties of Methylammonium Lead Iodide Perovskite, *Journal of Materiomics* (2015), doi: 10.1016/j.jmat.2015.07.005.

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**The Effect of the Surface Composition on Electronic Properties of
Methylammonium Lead Iodide Perovskite**

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Received date: 21 May 2015; Revised date: 9 July 2015; Accepted date: 15 July 2015

Abstract: Methylammonium lead iodide perovskite, $\text{CH}_3\text{NH}_3\text{PbI}_3$, is one of the most promising photovoltaic materials for low-cost and clean source of energy. In this work, the first-principles calculations were carried out to investigate the different composition of $\text{CH}_3\text{NH}_3\text{PbI}_3$ (001), including both methylammonium iodide terminated (MAI-T) and PbI_2 terminated (PbI_2 -T) surfaces. The calculated surface energies show that the MAI-T is thermodynamical more stable than the PbI_2 -T one under the equilibrium growth condition. The electronic properties of the two types of surfaces are also different. The band gap of PbI_2 -T is obviously smaller than that of MAI-T due to the surface Pb states. Band gaps of MAI-T decrease with increasing thickness, while band gaps of PbI_2 -T are insensitive to the slab thickness. The calculated optical absorption coefficients suggest that both terminations are effective solar energy absorbers in the visible light spectrum.

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