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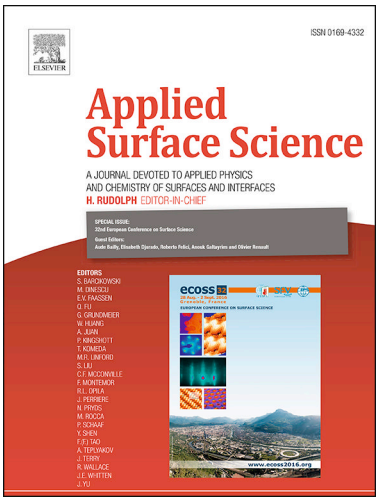

Full Length Article

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Zhenzhen Yang, Yuanxu Wang, Yunyan Liu

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Stability and charge separation of different $CH_3NH_3SnI_3/TiO_2$ interface: A first-principles study

Zhenzhen Yang[1], Yuanxu Wang[1,2]*, and Yunyan Liu[3,]*

[1]*Institute for Computational Materials Science, School of Physics and Electronics, Henan University, Kaifeng 475004, China*

[2]*School of Physics, Anyang Normal University, Anyang 455000, China*

[3]*School of Physics and Optoelectronic Engineering, Shandong University of Technology, Zibo 255049, China*

*Email: wangyx@henu.edu.cn, liuyunyan@sdut.edu.cn

ABSTRACT

Interface has an important effect on charge separation of perovskite solar cells. Using first-principles calculations, we studied several different interfaces between $CH_3NH_3SnI_3$ and TiO_2. The interfacial structure and electronic structure of these interfaces are thoroughly explored. We found that the SnI_2/anatase (SnI_2/A) system is more stable than the other three systems, because an anatase surface can make Sn-I bond faster restore to the pristine value than a rutile surface, and SnI_2/A system has a smaller standard deviation. The calculated plane-averaged electrostatic potential and the density of states suggest that SnI_2/anatase interface has a better separation of photo-generated electron-hole pairs.

Keywords: Perovskite solar cell; $CH_3NH_3SnI_3$ and TiO_2; Interface; first-principles