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Stability and charge separation of different $\text{CH}_3\text{NH}_3\text{SnI}_3/\text{TiO}_2$ interface: A first-principles study

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ABSTRACT

Interface has an important effect on charge separation of perovskite solar cells. Using first-principles calculations, we studied several different interfaces between $\text{CH}_3\text{NH}_3\text{SnI}_3$ and TiO_2 . The interfacial structure and electronic structure of these interfaces are thoroughly explored. We found that the $\text{SnI}_2/\text{anatase}$ (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 $\text{SnI}_2/\text{anatase}$ interface has a better separation of photo-generated electron-hole pairs.

Keywords: Perovskite solar cell; $\text{CH}_3\text{NH}_3\text{SnI}_3$ and TiO_2 ; Interface; first-principles

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