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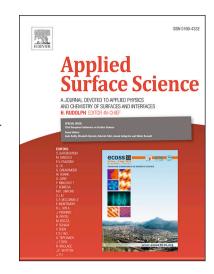
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Stability and charge separation of different CH₃NH₃SnI₃/TiO₂ interface: A first-principles study

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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 CH₃NH₃SnI₃ and TiO₂. The interfacial structure and electronic structure of these interfaces are thoroughly explored. We found that the SnI₂/anatase (SnI₂/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 SnI₂/A system has a smaller standard deviation. The calculated plane-averaged electrostatic potential and the density of states suggest that SnI₂/anatase interface has a better separation of photo-generated electron-hole pairs.

Keywords: Perovskite solar cell; CH₃NH₃SnI₃ and TiO₂; Interface; first-principles

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