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Exploring the Applicability of Un-doped and Doped Rutile TiO2 in Lead-Free Perovskite Solar Cells

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Abstract

On pure and metal, non-metal, co-doped rutile TiO2, DFT simula- tions are performed. For the stability study of doped materials, the defect formation energies of non-metal (S), metal (Fe), and metal and non-metal (Fe/S) co-doped materials are determined. A Ti- rich environment is preferable over an O-rich environment. With values of 2.98 eV, 2.18 eV, 1.58 eV, and 1.40 eV, the bandgap for pristine, S-doped, Fe-doped, and Fe/S co-doped materials is found to be direct. The effective masses (m*) and ratios (R) of charge carriers are also examined, and it is discovered that Fe/S co-doped material has the lowest charge carrier recombination rate. The maximum static dielectric constant is found in the Fe/S co-doped material. Doped material's absorption spectra shifted into the vis- ible region. Additionally, using SCAPS-1D simulation software, a complete solar cell device study using these materials as ETL is performed for the first time. The absorber layer and the ETL settings have been tweaked to perfection. Current-voltage (IV) characteristics, quantum efficiency (QE), capacitance-voltage (CV) characteristics, and capacitance-frequency (Cf) character- istics are provided for optimize solar cells.When the smallest degree of defect for each layer is taken into account, the solar cell with Fe/S co-doped ETL has the highest efficiency of 34.27%.

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