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Ferroelectric Tuning of Photocatalytic Water Splitting on Epitaxially-Strained $TiO_2/SrTiO_3$ Hetero-Structure JUN HEE LEE, ANNABELLA SELLONI, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — Using first-principles density functional theory (DFT) calculations, we show that the electric-dipole moment and epitaxial strain in heterostructures of TiO_2 with polar oxides such as $SrTiO_3$ can be used as control parameters to tune the activity of TiO_2 toward water splitting. Specifically, we find that the ferroelectric dipole of strained $SrTiO_3$ rigidly shifts the band-edge-energy positions of epitaxial TiO_2 films and affects the adsorption of relevant species (OH, H) on the TiO_2 surface. By varying the magnitude of the electric dipole moment and epitaxial strain, this effect can facilitate the oxygen evolution reaction and hydrogen production on TiO_2. In particular, our results show that a positive electric dipole pointed toward TiO_2 and compressive epitaxial strain can strongly reduce the barrier for oxygen evolution and thus significantly enhance the photocatalytic efficiency of TiO_2.

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