TiO_2/Ferroelectric Heterostructures as Polarization-Promoted Catalysts for Water Oxidation

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Using density functional theory calculations, we study the chemical activity of epitaxial heterostructures of TiO_2 anatase on strained polar $SrTiO_3$ films focusing on the oxygen evolution reaction (OER), the bottleneck of water-splitting. The reactivity of the TiO_2 surface is tuned by electric dipoles dynamically induced by the adsorbed species during the intermediate steps of the reaction while the initial and final steps remain unaffected. Compared to the OER on unsupported TiO_2, the combined effects of the dynamically induced dipoles and epitaxial strain strongly reduce rate-limiting thermodynamic barriers and significantly improve the efficiency of the reaction.