

Abstract Submitted
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On the Role of Fe₂O₃ Surface States for Water Splitting MAYTAL CASPARY TOROKER, Department of Materials Science and Engineering, Technion - Israel Institute of Technology — Understanding the chemical nature and role of electrode surface states is crucial for improved electrochemical cell operation. For iron (III) oxide (α -Fe₂O₃), which is one of the most widely studied anode electrodes used for water splitting, surface states were related to the appearance of a dominant absorption peak during water splitting. The chemical origin of this signature is still unclear and this open question has provoked tremendous debate. In order to pin down the origin and role of surface states, we perform first principle calculations with density functional theory +U on several possible adsorbates at the α -Fe₂O₃(0001) surface. We show that the origin of the surface absorption peak could be a Fe-O•type bond that functions as an essential intermediate of water oxidation

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