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Energetic and solvation effects at photoanode-catalyst interfaces: IrO2/WO3[1] YUAN PING, Joint Center for Artificial Photosynthesis, California Institute of Technology and Lawrence Berkeley National Laboratory, WILLIAM GODDARD III, Joint Center for Artificial Photosynthesis, California Institute of Technology, GIULIA GALLI, The University of Chicago — One key challenge in building photo-electrochemical cells to split water is to engineer interfaces between photo-electrodes and catalysts that are stable in harsh pH conditions and permit optimal charge transfer. Iridium oxide is the only known catalyst for oxygen evolution stable in acidic conditions and hence a good candidate to be interfaced with photoanodes. Using ab initio calculations, we investigated the structural and electronic properties of tungsten trioxide surfaces interfaced with an iridium dioxide thin film. We built a microscopic model of the interface that exhibits a formation energy lower than the surface energy of the most stable IrO2 surface, in spite of a large lattice mismatch, and we found no impurity states pinning the Fermi level. Both within Density Functional and many body perturbation theory (GW), we found that the two oxides form undesirable Ohmic contacts, when an IrO2 thin film fully covers WO3. However, our calculations predicted that if the morphology of the catalyst allows for partial exposure of the two oxides to water, then Schottky barriers may be formed, which favor charge transfer and hence water splitting. This work suggests ways to optimize light-absorber-catalyst interfaces for optimal charge transport.

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