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Band offsets across solid-liquid interfaces from continuum solvation methods[1] RAVISHANKAR SUNDARARAMAN, YUAN PING, GIULIA A. GALLI, WILLIAM A. GODDARD III, Joint center for artificial photosynthesis, CA — The band edge positions of photo-electrodes relative to water redox potentials play an important role in determining the efficiency of the photo-electrochemical cell. Direct theoretical calculations of solid-liquid interfaces are expensive and simplified models are desirable for rapid theoretical screening of new materials. However, traditional solvation models are extensively fit to describe organic solutes and hence extrapolate poorly to highly-polar inorganic surfaces. We develop minimally-empirical continuum solvation models suitable for treating such surfaces[2,3] and present theoretical predictions of the band positions of rutile TiO2 (110) and WO3 (001) surfaces in water. We obtain non-negligible solvation effects $\sim$ 1-2 eV, in good agreement with experimental results.[4,5,6,7]

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