Title:

Water Oxidation Catalysis with Fe_2O_3 Constrained at the Nanoscale

Abstract:
Photoelectrochemical cells containing iron(III) oxide (Fe_2O_3) have attracted extensive investigations due to their ability to convert solar energy into chemical energy by water splitting. Recently, fabrication of nanoscaled Fe_2O_3 has been adopted for photoelectrochemical cells to increase solar energy absorption and reduce slow diffusion length of charge carriers. To understand how nanoscaled confinement influences catalytic efficiency, we perform density functional theory + U calculations of water oxidation on a thin slab of Fe_2O_3(0001). We consider possible hydrogen vacancies that may appear at high pH and voltage and find that promoting hydrogen vacancy formation improves catalytic efficiency. We also analyze the effect of geometrical strain on the slab that may result from deposition on a substrate. We conclude that nano-Fe_2O_3 should be grown on a substrate with a similar lattice constant to reduce strain and improve catalytic efficiency.