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Water interaction and dissociation on the (0001) hematite surface: A DFT+U approach

Fabio R Negreiros and **Gustavo M Dalpian**
Federal University of ABC, Brazil

Statement of the Problem: A great deal of attention has been devoted to the study of photocatalytic effects on the interface between insulating oxide materials and water. It has been widely demonstrated for a variety of materials that water splitting can occur at these surfaces under certain specific conditions. The choice of the best material includes a balance between cost and performance. Among the desired properties, we need a specific band gap and band offset in order for the oxidation and reduction energies of water to be placed inside the band gap. There has been considerable interest in hematite, owing to its low cost and good photocatalytic activity. A considerable amount of theoretical and experimental works characterizing this structure can be found in the literature. The interaction of hematite with water is, therefore, of great interest for both academic and industrial purposes.

Methodology & Theoretical Orientation: We performed DFT+U calculations to study the interaction of water with the Fe_2O_3 (0001) surface. Using the CP2K and QE open source softwares, we determined the most stable configurations of a single water molecule adsorbed on the pristine oxygen-terminated surface, and how adding more water changed this interaction. Surface oxygen and iron vacancies were also considered at different charge states.

Findings: *Ab-initio* molecular dynamics simulations at room temperature reveal that water spontaneously dissociates ($H_2O \rightarrow H+OH^-$) at the interface, covering more than 50% of the surface with hydroxyls. Furthermore, in oxygen rich conditions, surface iron vacancies are found to be more stable than the pristine surface as long as the electronic chemical potential is 1 eV higher than the Fermi energy. Iron vacancies also increase the water dissociation rate at the interface.

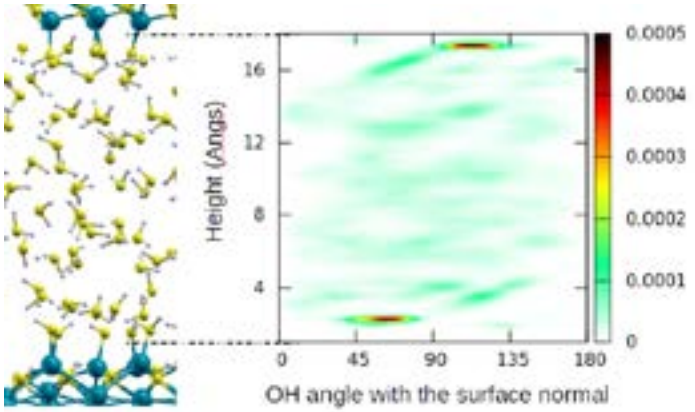

Figure: Water dissociates at the interface at 300K. The distribution of the angles between OH and the surface normal is shown on the right. Fe/O/H atoms are in cyan/yellow/white, respectively.

Biography

Fabio R Negreiros has his expertise in Computational Physics applied in condensed matter physics. His main areas of research are "Surface physics, heterogeneous catalysis and reactivity of metal and oxides surfaces in catalysis". He has developed scripts that apply global optimization techniques at DFT level, calling both CP2K/QE packages.

f.ribeiro@ufabc.edu.br