

Abstract Submitted
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Water Dissociation on the 0001 Hematite Surface¹ FABIO NEGREIROS RIBEIRO, Federal University of ABC, LUANA S. PEDROZA, GUSTAVO M. DALPIAN TEAM — Hematite is one of the many types of iron oxide that is easily found in nature. It is most commonly used in catalysis and it is rarely present in its pristine form. The influence of charged defects in its properties is very important for the correct geometrical/electronic characterization in more realistic operative conditions. Its interaction with water is also interesting for both academic and industrial purposes. In this work we performed DFT+U calculations to study water dissociation on the $Fe_2O_3(0001)$ surface using the CP2K software. We first determined the most stable configurations of a single water molecule adsorbed on the surface with and without oxygen/iron vacancies, considering also the charge state of each defect. The energy for the water molecule dissociation in O^{2-} and two protons was evaluated for each case, and it was found that the surfaces presenting iron vacancies are the most efficient ones for such process. In a second step we performed a few ab-initio molecular dynamics simulations at room temperature with several water molecules to accurately determine the liquid water/hematite interface, highlighting how the defects and the charge state change this interface.

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