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Effect of charges on the interaction of water with hematite[1] FABIO NEGREIROS RIBEIRO, LUANA PEDROZA, GUSTAVO DALPIAN, Universidade Federal do ABC — 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, but very few studies focus explicitly on these defects in this system. In this work we perform first principles DFT+U calculations to determine the properties of a hematite slab when both dopant and electrons/holes are added. We focus on the differences between the geometrical/electronic properties between the neutral/charged surfaces and also study their interaction with water (molecule and liquid) by performing molecular dynamics simulations at room temperature. Our results indicate that electric charges strongly influence the properties of these surfaces, changing the binding energies and the molecular arrangement of the water molecules adsorbed on hematite. Negative charges induce a larger binding and favor the partial water dissociation, whereas positive charges weaken the binding energy. We will provide comparative results for different configurations of this system.

[1]FAPESP

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