Abstract Submitted
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Density-functional study of chemical reactions at a solid-fluid interface: passivation of the (0001) surface of Cr_2O_3 SAHAK PETROSYAN, Department of Physics, Cornell University, ANGELIKI RIGOS, Department of Chemistry, Merrimack College, TOMAS ARIAS, Department of Physics, Cornell University — Using a new form of density functional theory for the *ab initio* description of electronic systems in contact with a dielectric environment, we present the first detailed study of the impact of a solvent on the surface chemistry of Cr_2O_3, the passivating layer of stainless steel alloys. Compared to vacuum, we predict that the presence of water has little impact on the adsorption of chloride ions to the oxygen-terminated surface but a dramatic effect on the binding of hydrogen to that surface. These results indicate that the dielectric screening properties of water are important to the passivating effects of the oxygen-terminated surface.

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