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Fe adsorption on the hematite (0001) and magnetite (111) surface¹ ADAM KIEJNA, TOMASZ PABISIAK, Institute of Experimental Physics, University of Wrocław, Wrocław — A detailed ab initio investigation of the structural, electronic and magnetic properties of Fe-atom adsorption on the hematite (0001) and magnetite (111) surfaces is presented. Spin-polarized density functional theory calculations are applied accounting for strong electron correlation effects by including a Hubbard-type on-site Coulomb repulsion (the DFT+U approach). For each oxide surface, the adsorption on two terminations has been studied: one terminated with Fe and the other with oxygen. The binding sites and coordination geometry of Fe adatoms are identified. Different adatom coverages were considered. The Fe atoms bind strongly to the Fe-oxide surfaces and induce large changes in their near surface geometry, and the electronic and magnetic properties. The binding of Fe is distinctly stronger at the O- than at the Fe-terminated surfaces of both oxides. The resulting adsorption energetics, structure and bonding are discussed based on the calculated local density of states and electron charge transfer.

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