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Partial dissociation of Water on Fe_3O_4 (001): Adsorbate Induced Charge and Orbital Order NARASIMHAM MULAKALURI, ROSSITZA PENTCHEVA, MARIA WIELAND, WOLFGANG MORITZ, Dept. of Earth and Environmental Sciences, University of Munich, Germany , MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — Besides potential applications in spintronics, magnetite plays an important role in many environmental redox reactions. Using density-functional theory together with an on-site Coulomb repulsion term (GGA+U), we investigate the interaction of water and its influence on the electronic properties and surface reconstruction of Fe_3O_4(001). The surface phase diagram, compiled within the framework of *ab initio* atomistic thermodynamics, reveals dissociative adsorption especially at surface defect sites. At higher water vapour pressures a partial dissociation sets in where a chain of hydrogen bonded H_2O and OH groups forms. The mixed adsorption mode and a suppression of the $(\sqrt{2}\times\sqrt{2})R45^\circ$ reconstruction is confirmed by a quantitative low energy electron diffraction analysis. The defects and adsorbates induce a unique charge and orbital order on the Fe_3O_4(001) surface[1].

1. N.Mulakaluri *et al.*, Phys. Rev. Lett **103**, 176102 (2009).

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