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Magnetic Anisotropy of Oxygen-deficient Fe/MgO(001) System: An ab Initio Study

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Using ab initio calculations, we study the MgO(001) and Fe/MgO(001) surface phases and the effects of interface structure on the Fe/MgO magnetic anisotropy. The surface phase diagrams of MgO(001) and Fe/MgO(001) show that the most stable surface structures are either defect-free surface or the surfaces with oxygen vacancies in c(2×1) periodicity for the systems. By the formations of the oxygen vacancy rows on MgO(001) surface, the in-plane magnetic anisotropy energy of Fe overlayer is reduced while the perpendicular magnetic anisotropy energy is increased from 0.1 to 0.5 meV per Fe atom.

Keywords: Magnetic anisotropy, Fe/MgO, DFT