S1-P002

Interface dependent magnetic anisotropy of Fe/BaTiO3(001): an ab initio study

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Using first principles calculations, we investigated the interface structure effects on the magnetic properties of the Fe/BaTiO3 system. On the BaO-terminated surface, a Fe monolayer is formed as two Fe atoms are adsorbed on the top sites of Ba and O in the (1×1) surface unit and a Fe ML is formed on the TiO2-terminated surface as two Fe atoms are adsorbed on the two O top sites. The magnetic anisotropy energy of Fe was higher on the TiO2?-erminated surface (1.5 eV) than on the BaO-terminated surface (0.5 eV). The decomposed electron density of the states showed that the stronger hybridization of Fe with the TiO2 layer than with the BaO layer is the most important reason for the higher magnetic anisotropy energy.

Keywords: DFT, Magnetism, Fe/BaTiO3, ab initio, magnetic anisotropy