d^0 Ferromagnetic Surface in HfO_2

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Recent theoretical studies have proposed a way to induce magnetism in simple oxides without containing magnetic transition metal ions (therefore, called d^0 magnetism). For instance, it has been proposed that a simple oxide such as CaO can be ferromagnetic with a small amount of cation vacancies. [1] It has been also shown theoretically that C- and N-doped CaO becomes ferromagnetic and half metallic. [2] Here, we propose another pathway to induce d^0 magnetism in simple oxides with no magnetic ions involved. First principles simulations based on density functional theory are performed to study surface magnetic properties of low index cubic, tetragonal, and monoclinic HfO_2 surfaces with different terminations. Our systematic calculations reveal that only O rich non-stoichiometric surfaces can be ferromagnetic. The origin of ferromagnetism found here is attributed to O surface electronic states with large O $2p$ spin exchange energy. We also discuss a possible reason for recent controversial experimental observations of ferromagnetism in HfO_2.

[1]I. S. Elfimov, S. Yunoki, and G. A. Sawatzky, *Phys. Rev. Lett.*, **89**, 216403 (2002).
[2]K. Kenmochi, *et al.*, *Jpn. J. Appl. Phys., Part 2* **43**, L934 (2004).