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Can pristine semiconducting oxides be ferromagnetic? HOA HONG NGUYEN, Laboratoire LEMA, UMR 6157 CNRS, Université F. Rabelais, Tours, France, A. BARLA, CELLS-ALBA, Barcelona, Spain, J. SAKAI, Lab. LEMA, QUE HUONG NGUYEN, Marshall University, Huntington, WV 25701
— The recent finding of FM in HfO_2 thin films of Coey's group has urged us to re-judge the role of TM doping in introducing FM into semiconducting oxides. Our observation of FM in undoped TiO_2, HfO_2, In_2O_3, ZnO, and SnO_2 confirmed that magnetism is possible in pristine oxide thin films, and FM is likely due to oxygen vacancies. This assumption is confirmed by our XMCD measurement on TiO_2 films: The FM in TiO_2 films is indeed intrinsic, and stems from both O-2p and Ti-3d electrons. In semiconducting oxides, the origin of magnetism is not due to the doping, but oxygen vacancies/defects. A big issue is how to find a more appropriate model to explain better the mechanism. We propose a model based on an electronic structure calculation using the tight binding method in the confinement configuration. Vacancy sites in TiO_2, HfO_2, In_2O_3 films could create spin splitting and high spin state, so that the exchange interaction between the electrons surrounding the oxygen vacancy with the local field of symmetry could lead to a FM ground state. Calculations give the results of 3.18 μ_B/vac for TiO_2, 3.05 μ_B /vac for HfO_2 and 0.16 μ_B /vac for In_2O_3. This model suggests that confinement effects play an important role in shaping up magnetic properties of low dimension systems.

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