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Intrinsic Defect Ferromagnetism: The case of Hafnium Oxide CHAITANYA DAS PEMMARAJU, STEFANO SANVITO, Trinity College, Dublin-2, Ireland — In view of the recent experimental reports of intrinsic ferromagnetism in Hafnium Oxide (HfO_2) thin film systems [1], we carried out first principles investigations to look for magnetic structure in HfO_2 possibly brought about by the presence of small concentrations of intrinsic point defects. *Ab initio* electronic structure calculations using Density Functional Theory (DFT) show that isolated **cation** vacancy sites in HfO_2 lead to the formation of high spin defect states which couple ferromagnetically to each other. Interestingly, these high spin states are observed in the low symmetry monoclinic and tetragonal phases while the highly symmetric cubic flourite phase exhibits a non-magnetic ground state. Detailed studies of the electronic structure of cation vacancies in the three crystalline phases of Hafnia show that symmetry leading to orbitally degenerate defect levels is not a pre-requsite for ferromagnetism and that the interplay between Kinetic, Coulomb and Exchange energy together with favourable coupling to the Crystalline environment can lead to high spin ferromagnetic ground states even in extreme low symmetry systems like monoclinic HfO_2. These findings open up a much wider class of systems to the possibility of intrinsic defect ferromagnetism.

[1]M. Venkatesan, C. B. Fitzgerald, J. M. D. Coey Nature **430**, 630 (2004) Brief Communications

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