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Search for ferromagnetism in transition metal doped ZnO nano-clusters¹ INDRA DASGUPTA, Department of Solid State Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, India, NIRMAL GANGULI, Department of Solid State Physics, Indian Association for the Cultivation of Science, Calcutta 700 032, India , BIPLAB SANYAL, Department of Physics and Materials Science, Uppsala University, Uppsala, Sweden — We present a comprehensive study of the energetics and magnetic interactions in 3d transition metal doped ZnO clusters by ab-initio density functional calculations. We find an important evidence that the charge state of the dopant transition element located at the surface of the cluster is different from that expected in the bulk and has a crucial impact on their magnetic properties. In addition, our calculations clearly reveal defects namely Zn and O vacancies in ZnO in neutral and charged states can induce ferromagnetic interactions between the transition metal atoms whereas anti ferromagnetic coupling dominates in a neutral defect-free cluster. Our results can have significant contributions in the nano-engineering of defects to achieve desired ferromagnetic properties in spintronics applications.

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