Abstract Submitted
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Non-stoichiometric Mn doped ZnO clusters: First principles calculations[1] SACHIN P. NANAVATI, SHAILAJA MAHAMUNI, S.V. GHAISAS, University of Pune, India, VIJAY KUMAR, Dr. Vijay Kumar Foundation, Gurgaon, India — It has been reported that cage like hollow clusters of $(ZnO)_n$ with $n = 12$ & 34 are stable and hence *magic*. Doping Mn impurity in ZnO (ZnO:Mn) clusters is a well studied problem. In most of the studies, single Mn doping has been achieved by substituting it on a surface Zn site, leading to a stoichiometric configuration of $Zn_{n-1}MnO_n$ and a large magnetic moment of 5 μ_B. However, we show that using first principles methods, Mn doping would lead to O rich, non-stoichiometric clusters with significantly reduced magnetic moment. Specifically, we show that clusters of configuration $Zn_{12}MnO_{15}$ and $Zn_{34}MnO_{37}$, obtained when Mn is substituted in $(ZnO)_n$ ($n = 13$ & 35) cages, become magic. The magnetic moments in these clusters is reduced to 1 μ_B. These clusters can also be considered as a composite structure where a MnO_x ($x = 1$ to 4) molecule is attached to ZnO_n ($n = 12$ & 34) cages from outside.[2] We believe that these results would have important implications for the understanding of magnetism in ZnO:Mn nanostructures as well as thin films, for which recent experiments suggest mixed and higher oxidation states of Mn, *viz.,* Mn^{+3} and Mn^{+4}.

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[2]S. P. Nanavati et al. Phys. Rev. B (in press, 2012).

S. P. Nanavati
Dept. of Electronic Science, University of Pune, Pune 411007, India

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