Abstract Submitted
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**Magnetism in transition doped ZnO** PRIYA GOPAL, NICOLA SPALDIN, Department of Materials, UCSB — We present results of our detailed density functional investigation of ZnO doped with a series of *3d* transition metal ions (Cr, Mn, Fe, Co, Ni and Cu). We have calculated the strength of the magnetic interactions when a single atom type is used as a dopant as well as the effects of simultaneous doping with two different transition metal ions. In addition, we have also done simulated *p*-type doping in ZnO by substituting one of the Zn atoms by the monovalent ions , $Li^+$ and $Cu^+$ and determined the influence on the magnetism. We have also introduced defects in the form of O and Zn vacancies and its effect on magnetism. We find that our results are highly sensitive to the details of the calculations, including energy and k-point convergence, structural optimization and choice of exchange-correlation functional. However, our highly converged results suggest that above room-temperature ferromagnetism is not possible in transition metal doped ZnO without additional carriers and the experimental reports of high temperature ferromagnetism in this system could be due to the presence of secondary phases.

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