

Abstract Submitted
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Magnetism and Energetics of Mn Doped ZnO (10 0) Thin Film

BIJAN K. RAO¹, QIAN WANG, PURU JENA, Virginia Commonwealth University
— First principles calculations based on gradient corrected density functional theory are performed on Mn doped ZnO thin film. Magnetism and energetics are studied for two Mn concentrations and varying Mn configurations. It is found that in the dilute limit when Mn atoms are far apart, the ferro- and anti-ferromagnetic states are energetically nearly degenerate. The resulting fluctuation would, therefore, make the system paramagnetic as found in the experiment. But, as the concentration of Mn atoms increases, there is a tendency for Mn atoms to form nearest neighbors and cluster around oxygen. For such a configuration, the anti-ferromagnetic coupling between Mn atoms is energetically more favorable. The results are compared with a diverse range of experiments on Mn doped ZnO thin film.

¹Deceased

Puru Jena
Virginia Commonwealth University

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