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Transition Metal Doped and Encapsulated ZnO Cages MARCELA

R. BELTRAN, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, ARTHUR REBER, SHIV N. KHANNA, Physics Department, Virginia Commonwealth University — ZnO is a wide band gap semiconductor with potential for applications. We had earlier shown that $Zn_{12}O_{12}$, $Zn_{15}O_{15}$, $Zn_{18}O_{18}$, and $Zn_{21}O_{21}$ clusters are particularly stable and exhibit cage structures. In this work, we examine the possibility of making magnetic materials by either substituting Zn atoms by transition metal atoms or by encapsulating transition metal clusters inside the cages. Our studies are carried out within a density functional framework employing gradient corrected functionals. The studies cover all the 3d elements and examine the strength of the magnetic moment as well as the nature of the coupling between the local moments. We also present results on the coupling between the endohedral transition metal cluster and the transition metal atoms substituting for Zn atoms within the cage.

Shiv N. Khanna
Physics Department, Virginia Commonwealth University

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