

Abstract Submitted
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Adsorption, Symmetry and Magnetic Properties in TM-GaN Nanocrystals¹ HAIBIN HE, YAN DONG, KEMING FU, MING JIANG², Dept. of Physics, Yantai University, P.R. China — Transition metal(TM)-doped dilute magnetic semiconductor nanocrystals are of interest for potential applications in spintronics due to their tunable properties. The physical properties of semiconductor nanocrystals depend on their size or shape. we present first-principles calculations for the electronic structure and magnetic properties of completely passivated, H- adsorbed and isolated Mn/Cr-doped GaN nanocrystals with different point symmetry. A novel half-metallicity and magnetic metastability has been found. The multiple metastable spin states and spin-flip for metallic channel are demonstrated in these nanocrystals with the various H coverages and point groups symmetry. A detailed electronic structure analysis is given. Our calculated results imply a new type of half-metallic and spin-crossover nanomaterial.

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²Corresponding Author

Ming Jiang
Dept. of Physics, Yantai University, P.R. China

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