Electronic and magnetic properties of Mn-doped ZnO:

Total-energy calculations

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Abstract

Based on the spin generalized gradient approximation (**σ**GGA) of the density functional theory (DFT), the structural, magnetic, and electronic properties of Mn-doped ZnO structure have thoroughly been investigated. It is found that the Mn atom prefers to substitute one of the Zn atoms, producing the energetically most stable configuration for the Mn-doped ZnO structure. Employing the Hubbard potential within the calculations suggests various changes and modifications to the structural, magnetic and electronic properties of the Mn-doped ZnO. Our calculations reveal that the local magnetic moment at the Mn site using the ordinary **σ**GGA functional is 4.84 μ_B/Mn, which is smaller than that evaluated by including the Hubbard potential of 5.04 μ_B/Mn. Overall, the electronic band structure of the system, within the **σ**GGA+U, is half-metallic, with metallic nature for the majority state and semiconducting nature for the minority state. Simulated scanning tunneling microscopy (STM) images for both unoccupied and occupied states indicate siginficant brightness on both Zn and Mn atoms and much brighter protrusions around the O atoms, respectively.

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