Electronic Structure and Ferromagnetism of Mn Implanted n- and p-type ZnO.

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The prediction of room temperature magnetism in Mn doped ZnO has generated considerable interest in this compound, both from the experimental and theoretical point of views. In order to take into account the strong on-site correlations of the rather localized d-electrons, we use the self-interaction corrected (SIC)-LSD approximation. Within this scheme, the 3d electron manifold is considered to consist of both localized and itinerant states, both of which are treated on an equal footing, by adding a contribution for each d-electron to localize. By varying the relative proportions of localized and delocalized states, the most favorable (ground state) configuration can be established. Our calculations show that the 3d electrons in Mn doped ZnO prefer to localize. We furthermore have studied the effects on the electronic structure, when $Zn_{1-x}Mn_xO$ is codoped with N atoms (n-type ZnOMn), and Ga and Sn atoms (n-type ZnOMn) respectively.

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