First-Principles Studies of Magnetic Properties of ZnO-based DMSs

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Currently ZnO-based materials have been receiving considerable attention due to their potential applications in spintronics, light-emitting diodes, laser diodes, UV detectors, cosmetics and biomaterials. The novel magnetic, electronic, optical, and electro-mechanical properties of ZnO offer the unique possibility to create multi-functionally integrated devices for sensing, processing, and actuating functions in one monolithic structure. For spintronic applications, the design of a transparent piezoelectric dilute magnetic semiconductor (DMS) has been pursued through a small amount doping of a transition metal (TM) ions in ZnO. However, experimental works on exploring the magnetism of ZnO-based DMSs have been highly conflicting. Using first-principles theory and band structure methodology we have systematically studied the electronic structure and magnetic properties of TM-doped ZnO (TM=V, Cr, Mn, Fe, Co, and N) in bulk as well as thin films. Our results suggest that ferromagnetic $Zn_{1-x}TM_xO$ thin film with Cr, Mn, Fe, Co or Ni substituting Zn sites is difficult to achieve without further modification. We have also studies the dependence of the magnetic coupling on the type and concentration of defects. Especially we have successfully predicted that the ferromagnetism in Mn-doped ZnO can be realized through N co-doping, which has been confirmed by many recent experiments. Our study provides a general understanding of the magnetic coupling between TM ions in ZnO-based DMSs.

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