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Structural and Magnetic Properties of Transition-Metal-Doped $Zn_{1-x}Fe_xO$

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The ability to produce high-quality single-phase diluted magnetic semiconductors (DMS) is the driving factor to study DMS for spintronics applications. Fe-doped ZnO was synthesized by using a low-temperature co-precipitation technique producing $Zn_{1-x}Fe_xO$ nanoparticles (x = 0, 0.02, 0.04, 0.06, 0.08, and 0.1). Structural, Raman, density functional calculations, and magnetic studies have been carried out in studying the electronic structure and magnetic properties of Fe-doped ZnO. The results show that Fe atoms are substituted by Zn ions successfully. Due to the small ionic radius of Fe ions compared to that of a Zn ions, the crystal size decreases with an increasing dopant concentration. First-principle calculations indicate that the charge state of iron is Fe^{2+} and Fe^{3+} with a zinc vacancy or an interstitial oxygen anion, respectively. The calculations predict that the exchange interaction between transition metal ions can switch from the antiferromagnetic coupling into its quasi-degenerate ferromagnetic coupling by external perturbations. This is further supported and explains the observed ferromagnetic behavior at magnetic measurements. Magnetic measurements reveal that decreasing particle size increases the ferromagnetism volume fraction. Furthermore, introducing Fe into ZnO induces a strong magnetic moment without any distortion in the geometrical symmetry; it also reveals the ferromagnetic coupling.