Multifunctional Nanostructured Co-doped ZnO: The Co Spatial Distribution and the Correlated Magnetic Properties

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There is a huge technological interest in the development of functional nanostructured systems. In this context, doping strategies, as for bulk materials, have been explored in order to tailor and improve the properties in a desired way to allow its applicability in useful and commercial devices. However, at nanoscale, quantum mechanical effects leads to new phenomena that at the same time can hinder the achievement of specific targets and be used to develop new functionalities that cannot be implemented in bulk systems. Here, in this report we present a systematic structural and magnetic analysis of Co-doped ZnO nanoparticles prepared via a microwave-assisted hydrothermal route. The structural data confirm the incorporation of Co ions into the wurtzite ZnO lattice and a Co concentration mainly near/at the surface of the nanoparticles. This Co spatial distribution is set to passivate the surface of the ZnO nanoparticles, inhibiting the nanoparticle growth and suppressing the observation of a ferromagnetic phase. Based on experimental and theoretical performed via first-principles calculations based on density functional theory (DFT) results, we propose a kinetic-thermodynamic model for the processes of nucleation and growth of the Co-doped ZnO nanoparticles, and attribute the observed ferromagnetic order to a ferromagnetism associated with specific defects and adsorbed elements at the surface of the nanoparticle. Our findings give valuable contribution to the understanding of both the doping process at the nanoscale and the nature of the magnetic properties of the Co-doped ZnO system.
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