

# Investigation of Structural, Morphological, and Photoluminescence Properties of $Zn_{1-x}Mg_xS$ Nanoparticles Prepared by Solvothermal Method: Insight from Experimental and DFT Study

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**Abstract:** Various concentrations of  $Mg^{2+}$  substitutional doped ZnS nanoparticles ( $Zn_{1-x}Mg_xS_{,x} = 0, 0.02, 0.07, \text{ and } 0.1$ ) were prepared by adopting the solvothermal method, using ethanol as the solvent at  $135^\circ\text{C}$ . The obtained micro/nanoparticles were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and room temperature photoluminescence (PL) spectroscopy. XRD revealed the conservation of the host ZnS crystal phase after the substitution of  $Zn^{2+}$  by  $Mg^{2+}$  but was accompanied by a weak decrease of the lattice parameter. SEM analysis showed the formation of aggregated particles that were evenly distributed. PL spectra exhibited a near-band-edge (NBE) emission centered at 430 nm, and another band at 585 nm, related to sulfur defects; moreover, no shift occurred when  $x$  increased. To explain this finding, computational density functional theory (DFT) calculations were performed, revealing constant gap energy after substitution was maintained at the point G, whereas the density of states of both CV and BV were reinforced near the band gap

**Keywords :** solvothermal preparation,  $Zn_{1-x}Mg_xS$  substitution doped, structural study, Photoluminescence (LP), DFT calculations