Russian Journal of Physical Chemistry A

Volume 97, Issue 8, 2023, Pages 1769-1778

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

Messai Youcef, Bezzi Hamza, Bourzami Riadh, Chetoui Abdelmounai, Bouarroudj Tayeb, Samira TLILI, Tairi Latifa, Ahmed Belghidoum, Ouksel Louiza

Abstract: Various concentrations of Mg^{2+} substitutional doped ZnS nanoparticles ($Zn_{1-x}Mg_xS_{,x}$ = 0, 0.02, 0.07, and 0.1) were prepared by adopting the solvothermal method, using ethanol as the solvent at 135°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 stats of both CV and BV were reinforced near the band gap

Keywords : solvothermal preparation, Zn1-xMgxS substitution doped, structural study, Photoluminescence (LP), DFT calculations