COMBINED EXPERIMENTAL AND DFT STUDY OF LITHIUM-INDIUM-OXIDE STRUCTURE AND VIBRATIONAL PROPERTIES

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Abstract

A promising lithium-indium-oxide ($LiInO_2$) wide band-gap semiconductor for scintillating detection, photoluminescence, and photocatalysis [1-3] was prepared by a mechanochemical solid-state synthetic procedure that can be found elsewhere [3]. Its structure and morphology were investigated by using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Raman spectroscopy. SEM images show agglomerates of relatively uniform size of around 300 nm spherical-shaped particles of $LiInO_2$ powder, while the XRD pattern confirmed the formation of the nanocrystalline tetragonal structure with $I4_1/amd$ space group (no. 141) symmetry. Detailed vibration analysis, together with the assignments of the band modes, was performed through the best-fit match of the experimental and density functional theory (DFT) calculated Raman spectrum. Geometry optimizations and vibrational frequencies calculations were conducted using B97-1 functional correlation [4] and LanL2DZ was used as a basis set.

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