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Synthesis and characterization of NaMgF3:La2O3 NPs

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Recently, interest in lanthanum as a dopant in host materials has increased due to its ability to significantly modify the optical and structural properties of its host material. Fluoride nanocrystals doped with rare earth ions are of great interest due to their potential applications in lighting and displays, boost converters, biological fluorescent labels, transparent glass, scintillators, optical amplifiers, solar cell amplification and photodynamic therapy. The NaMgF3 material have been considered an ideal host for getting up- and down-conversion emission. The luminescence properties of Ln-doped NaMgF3 have revealed that the fluoroperovskite host is an excellent compound through which spectral information on various divalent lanthanides may be obtained. In this study $NaMgF_3$ doped with La_2O_3 rare earth oxide in a mass ratio of 1:0.2 was synthesized through co-precipitation and solid-state reaction (700℃, 6h). The X-ray diffraction pattern was recorded to check the phase purity of the synthesized compound. In order to identify the functional groups, the Fourier Transform Infrared spectral analysis have been performed. Chemical composition of the synthesized compounds was checked by the energy - dispersive X-ray spectra. XRD analysis of undoped $NaMgF_3$ exhibits crystalline structure with grown crystallite size of 35.7 nm and a strain of 0.27%. Doping $NaMgF_3$ with La_2O_3 reduces the crystallite size to 34.5 nm, while lattice strain remains unchanged at 0.27%. The decrease in crystal size is influenced by the radius of its constituent ions. La^{3+} doping has no effect on strain, suggesting that La^{3+} ions (103.2 pm) are incorporated without significantly altering the lattice parameters, possibly due to their closer match with Na^+ ionic radius (102 pm). Analysis of the survey XPS spectra of $NaMgF_3$ and $NaMgF_3$:La_2O_3 in the whole binding energy region are discussed. XPS analysis of the O1s core level for $NaMgF_3$ and $NaMgF_3$ doped with La_2O_3 reveals distinct oxygen for undoped $NaMgF_3$, at 539.1 eV, 532.1 eV, 529.3 eV, and 529.5 eV, likely corresponding to surface hydroxyl groups or adsorbed water (539.1 eV), lattice oxygen in $NaMgF_3$ (532.1 eV), and oxygen in metal-fluoride or oxide-related bonds (529.3–529.5 eV). $NaMgF_3$:La_2O_3 shows peaks at 539.4 eV, 532.4 eV, and 529.9 eV, with slight shifts suggesting minimal lattice disruption by La^{3+} ions, possibly due to their similar ionic radius of Na^+. The shifts and peak position variations of all elements of the compound influenced the electronic structure and potentially enhancing physical properties. XPS analysis of the F1s core level for $NaMgF_3$:La_2O_3 reveals F1s peaks at 687.5 eV and 686.3 eV, with a slight shift to higher binding energy for the main peak and an slightly increase for the secondary peak, suggests minimal lattice perturbation by La^{3+} ions, consistent with its unchanged lattice strain (0.27%) and near-identical crystallite size (34.5 nm). Knowledge of the speciation of La3+ in the lattice of $NaMgF_3$ is essential to understand how they incorporate, since the local structure of the dopant and its homogeneity within the host, determine its optical properties.
Keywords: NaMgF3 and $NaMgF_3$:La_2O_3 NPs, X-ray Analysis, Composition.
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