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Name of the Scholar : Ishtihadah Islam

Name of the Supervisor : Prof. Azher Majid Siddiqui

Name of the Department/Centre : Physics

Topic of the Research : Synthesis, Characterization and physical properties of transition metal doped oxide semiconductors: Bulk and Nanostructures

In the present research work, we report the synthesis of $Mg_{0.95}Mn0_{.05}O$ nanostructures and the effect of incorporation of different transition metal dopants (cobalt, nickel, copper and iron) on the structural, optical, morphological and dielectric properties. After introducing the readers to the title and multi-dimensions of MgMnO and its synthesis procedures, we broadly discuss the output in three chapters. First we carry out the synthesis of $Mg_{0.95}Mn_{0.04}TM_{0.1}O$ (TM= Co, Ni, Cu) by auto-combustion method. The pristine $Mg_{0.95}Mn0_{.05}O$ from X-ray diffraction plots confirm the cubic crystal structure. The observed crystallite size was found to be 78.2, 67.02, 78.11 and 64 nm for pure, Co, Cu and Ni doped MgMnO, respectively. Purity of the samples from Raman analysis and the presence of magnesium oxide in all samples was established from FTIR results. Optical transmission spectrum shows that these samples are highly transparent in the UV-visible region. Dielectric characterization depicts a reasonable decrease in the dielectric constant ε` as function of improving frequency, which in turn confirms its dispersive nature.Secondly, we tried to investigate the pH and Fe concentrations on the size, structural and physical properties of $Mg_{0.95}Mn_{0.05-x}Fe_xO$ (x = 0, 0.04) nanostructures prepared by the same route and varying the pH of the solution. We observed the phase purity, size and size distribution of the nanoparticles from powder X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Irrespective of the pH, Rietveld refinement analysis of the XRD data revealed the single crystallographic cubic phases with MgO-type wurtzite structure (space group $Fm\bar{3}m$) along with a lattice parameter of 4.2121(8) Å for x = 0.0 and 4.2083(5) Å for x = 0.04. This change in lattice parameter with Fe doping is due to the smaller size of Fe^{2+} (78 pm) compared with Mn^{2+} (83 pm). The size of the nanoparticles increased monotonically from approximately 10 nm to ~ 16 nm for x = 0.0 and from~ 18 nm to ~ 23 nm for x = 0.04 with increasing pH. SEM micrographs of the powders displayed the highly agglomerated nanoparticles with porous and irregular morphology. Later, the solid-state reaction synthesis of $BaSn_{1-x}Mn_xO_3$ (x = 0.0 - 0.3) perovskite structures is presented. Heavy transition metal doping in powdered $BaSnO_3$was accomplished to investigate the structural, morphological, chemical and dielectric properties of synthesized samples. Single phase, cubic crystal formations from the structural properties and the formation of polygonal discs with nanoscale (~50 nm) dimensions from Transmission electron micrographs (TEM) are revealed. Elemental composition of the synthesized samples from the x-ray photoelectron spectroscopy (XPS) was confirmed. Optical properties demonstrate the pristine $BaSnO_3$ as an ultraviolet active material within the band gap 3.2 eV. The enhancement in visible light active mode was achieved via band gap tuning by proportional Mn-doping in parent material. DFT calculated electronic structures support the optical characteristics, where a gradual decrease in band gap and increase in ferromagnetic ordering with the increase in Mn-content and vice-versa was observed .