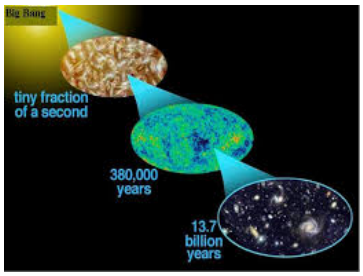

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Band gap engineering of barium stannate (BaSnO3) perovskite oxide by Mn-doping: Theory and experiment

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Band gap engineering of barium titanate (BaSnO3) perovskite oxide by Mn-doping: Theory and experiment

Ishtihadah Islam1, *Shakeel Ahmad Khandy2, Azher Majid Siddiqui1, Aurangzeb Khurram Hafiz3*
1Department of Physics, Jamia Millia Islamia, New Delhi 110025
2Department of Physics, National Taiwan University, Taipei, Taiwan
*3Centre for Nanoscience and Nanotechnology, Jamia Millia Islamia, New Delhi, 110025, India*ishtihadahislam@gmail.com

ABSTRACT
Nanocrystalline BaSn1-xMnxO3 (x = 0.0 - 0.3) nanostructures were synthesized by solid state reaction route. Heavy Mn-doping upto 30% in powdered BaSnO3 is accomplished to investigate the optical properties, electronic structure and magnetic properties of the synthesized samples. From XRD analysis and Transmission electron micrographs (TEM), nanoscale cubic structures are observed within (~50 nm) dimensions. Band gap transition from 3.2 eV in pure BaSnO3 to 2.6 eV in Mn-doped samples is coherent with DFT calculations. So, an ultraviolet active material is reduced to absorb the visible light via band gap engineering as achieved by proportional Mn-doping in the parent material. An increase in Mn-content leads to the decrease in band gap of parent material up to certain limits (20% doping only). The origin of these reduced values can be argued from the unpaired Mn-3d5 electronic states which induces the defect states below the conduction band minima near the Fermi level. The more, defect states present in a sample, the smaller will be its band gap. However, after certain doping (optimal 20% in present case), the distortion effects in the crystal structure does not allow further alteration of the band gap but induce magnetism only.

Keywords: BaSnO3; Nanoparticles, XRD, Transition metals, Optical properties

Primary author: ISLAM, Ishtihadah (Jamia Millia Islamia)

Presenter: ISLAM, Ishtihadah (Jamia Millia Islamia)