National Institute of Technology Rourkela

Defence Seminar

Seminar Title	: Atomic-level disorder and Microstrain in Near-Infrared Upconverting Core-Shell Nanocrystals due to Induced Lattice Defects
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Venue	: Seminar Hall, Chemistry Department (Hybrid mode: https://meet.google.com/spk-qnij-avj)
Date and Time	: 27 May 2025 (11.00 am)
Abstract	: With the emergence of strain-engineered nanostructured materials, understanding the nature of microstrain in nanoscale has become imperative. Since nanocrystals (NCs) exhibit complex strain influenced by crystal defects, the premise of studying atomic level disorder and its manifestation in microstrain and other physical properties of nanocrystals constitute a fundamental topic of research. In this dissertation, Nd^{3+}-containing NaYF4-based upconverting (UC) photoluminescent materials were studied as a model nanocrystal to investigate local disorder within a nanoparticle that is responsive towards 980 nm NIR excitation and capable of serving as a core nanocrystal for a core-shell (C-S) nano-construct responding to 808 nm NIR excitation. As a representative, core nanocrystals (13 nm) of NaYF4/Yb^{3+}/Tm^{3+}/Nd^{3+} were fabricated and Li^{+} ions were deliberately incorporated as a symmetry perturbing agent. Later, the same core NCs were covered with a single epitaxial layer of NaYF4/Nd^{3+} as a shell. Coherence between upconversion luminescence (UCL) intensity, atomic level disorder and microstrain was observed in the core NCs. While the atomic level disorder propagated in the same manner, the microstrain got reversed from core to C-S UCNCs. Such reversal of microstrain was studied with respect to the growth of the shell layer and interpreted in terms of lattice mismatch. Upon inducing lattice defects into the C-S systems by Li^{+}, the corresponding UCL intensity was maximized at some specific atomic disorder, where the tensile microstrain of C-S, compressive microstrain of the core, and atomic level disorders exhibited their respective extreme values irrespective of the activator ions. The study was supported by high-energy synchrotron X-ray (&lambda=0.568551 Å) diffraction (SXRD) coupled with the real space analysis of diffraction patterns using an atomic pair distribution function from the total X-ray scattering experiment, integral breadth calculation of SXRD data using the Williamson-Hall uniform deformation model, neutron diffraction, EXAFS, XANES, XPS, TEM and Rietveld refinement analysis of the diffraction patterns wherever required. This dissertation based-on high precision-experimental study refers to some fundamental understanding at nanoscale, paving the way for rational design of strain-engineered core-shell nanostructure.