Synthesis and Optoelectronic Characterizations of Cesium Tin Chloride Perovskite Nanocrystals

Speaker: Md. Shahjahan Ali (M.Sc. Student)

Abstract

In this investigation, thermally stable cubic phase cesium tin chloride ($CsSnCl_3$) perovskite nanocrystals were successfully synthesized with a promising surface morphology by adopting a rapid hot-injection technique. The excellent crystalline quality of these cubic shaped nanocrystals was confirmed by high resolution Transmission Electron Microscopy imaging. The binding of organic ligands on the surface of the as-prepared sample was identified and characterized by the Nuclear Magnetic Resonance spectroscopy. The UV-visible spectroscopy ensured that $CsSnCl_3$ nanocrystals have a direct band gap of ~2.98 eV which was further confirmed by Photoluminescence spectroscopy. The band edge positions calculated using the Mulliken electronegativity approach predicted the potential photocatalytic capability of the as-prepared nanocrystals which was then experimentally corroborated by the photodegradation of rhodamine-B dye under both visible and UV-visible irradiation. By employing experimental parameters, the electronic band structure, charge carrier effective masses etc. of $CsSnCl_3$ nanocrystals were calculated within the generalized gradient approximation (GGA) and GGA+U methods. The theoretical calculation demonstrated 90% accurate estimation of experimentally observed optical band gap when U_{eff} = 6 eV was considered. The ratio of the effective masses of the hole and electron expressed as $D = m_h^*/m_e^*$ was also calculated for U_{eff} = 6 eV. A rational interpretation of the "D" value was proposed based on this theoretical calculation and experimental observation of the photocatalytic performance of $CsSnCl_3$ nanocrystals. It is assumed that a "D" value of either much smaller or larger than 1 is the indication of low recombination rate of the photogenerated electron-hole pairs and the photocatalytic efficiency of a photocatalyst. This comprehensive investigation might be helpful for the large-scale synthesis of thermally stable cubic $CsSnCl_3$ nanocrystals and also for a greater understanding of their potential in photocatalytic and optoelectronic applications.