Smart Materials: Methods and Applications – 2017 (SMMA-2017) IL11

Defect Tolerant Cesium Lead Halide Perovskite Nanocrystals

Angshuman Nag

Department of Chemistry, Indian Institute of Science Education and Research (IISER), Pune 411008, India

Email: angshuman@iiserpune.ac.in

Defect tolerance signifies the tendency of a semiconductor to retain its electronic, optical and optoelectronic properties even in the presence of defects. Colloidal semiconductor nanocrystals like CdSe posses a notorious problem of surface defects, that trap charge carriers, severely limiting their properties. In this presentation, I will discuss our recent results suggesting defect tolerance behavior of cesium lead halide perovskite nanocrystals, where surface defects have minimal influence on the electronic, optical and optoelectronic properties.¹⁻⁶

Our colloidal CsPbBr₃ nanocrystals (11 nm) exhibit ~90% photoluminescence (PL) quantum yield with reduced blinking along with very high (~ 4500 cm²V⁻¹S⁻¹) carrier mobility (measured using THz spectroscopy) within a nanocrystal. These results suggest a near absence mid-gap deep trap states in these nanocrystals. This interesting behavior of cesium lead halide nanocrystal, where surface defects do not form trap states, originates from its unique electronic band structure where anti-bonding interactions of Pb 6s orbital with halide p orbitals forms the valence band maximum, and the conduction band minimum gets stabilized by spin-orbit coupling of Pb 6p states. Now we are exploring Pb-free metal halide nanocrystals.⁷

References:

- 1. Swarnkar, A; Chulliyil, R.; Ravi, V. K.; Irfanullah, M.; Chowdhury, A.; Nag A. Angew. Chem. Int. Ed. 2015, 53, 15424.
- 2. Yettapu, G. R.; Talukdar, D.; Sarkar, S.; Swarnkar, A.; Nag, A.; Ghosh, P.; Mandal, P. *Nano Lett.* **2016**, *16*, 4838.
- 3. Ravi, V. K.; Swarnkar, A; Chakravorty, R.; Nag,
- A. Nanotechnology **2016**, 27, 325708.
- 4. Ravi, V. K.; Markad, G. B.; Nag, A. ACS Energy Lett. 2016, 1, 665.
- 5. Mir, W. J.; Jagadeeswarara, M.; Das, S.; Nag, A. ACS Energy Lett., 2017, 2, 537.
- 6. Aneesh, J.; Swarnkar, A.; Ravi, V. K.; Sharma, R.; Nag, A.; Adarsh, K. V. J. Phys. Chem. C 2017, 121, 4734.
- 7. Swarnkar, A.; Ravi, V. K.; Nag, A. ACS Energy Lett., 2017, accepted. Perspective Article.