Poster Presentation

Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

"Structural and Photophysical Properties of $MA_xCs_{1-x}PbBr_3$ (x = 1, 0.5 and 0) Organic-Inorganic Hybrid Perovskites"

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Abstract: Organic-inorganic hybrid perovskite solar cells have attracted much attention due to their enormous potential in the future of photovoltaics. To date, the best perovskite solar cells are constructing by mixed organic cations [methylammonium (MA) and formamidinium (FA)] with mixed halides. Unfortunately, MA/FA compositions are sensitive to processing conditions because of their intrinsic structural and thermal instability. However, mixing of cesium (Cs) cation plays an important role to achieve higher thermal and structural stability of perovskites.

Present investigation has been carried out to understand the structural, photophysical and morphological properties of pure ($MAPbBr_3$, $CsPbBr_3$) and equimolar ratio of MA and Cs lead bromide ($MA_{0.5}Cs_{0.5}PbBr_3$) perovskites. The perovskites materials were synthesized by ligand-assisted re-precipitation (LARP) method. X-ray diffraction (XRD) has been utilized to investigate their structural properties, which reveal orthorhombic structure of all synthesized perovskites. Raman spectral analysis has been carried out to elucidate the effect of Cs in MA librational and torsional modes. The broad and unresolved band at 200-340 cm^{-1} is assigned to the torsional mode of the MA cations, and we proposed this mode as a possible marker of the orientational order of the organic cations in the materials. The morphology and particle size distribution have been predicted by the FESEM and TEM images. Further, thermal behavior of synthesized perovskites was performed by thermogravimetric analysis (TGA). The weight loss peaks at ~350, and 600 °C for $MA_{0.5}Cs_{0.5}PbBr_3$ and $MAPbBr_3$ perovskites can be assigned to a loss of organic ligands and inorganic framework, respectively. UV-Vis and photoluminescence (PL) spectra have been recorded to explore the optical properties. To determine the PL mechanism of the perovskites, PL decay curves were recorded; where a band edge emission with a short PL lifetime and a defect-related emission with a long PL lifetime were observed. For homogeneously synthesized perovskites, a shorter PL lifetime of ~1-4 ns was observed. These results suggest that the PL of synthesized perovskites is dominated by band edge emission. No defect-related emission was observed on PL and PL decay curves.

We believe the present study to provide the required assignments for the interpretation of the Raman spectra of perovskites, which may be extremely useful to understand in detail the properties of this class of materials in relation to their full exploitation in solar cells.

References and Notes:

1. (a) *Angew. Chem. Int. Ed.* **2017**, *56*, 14187; (b) *Nature* **2016**, *536*, 312; (c) *Proc. Natl. Acad. Sci. USA* **2016**, *113*, 11694; (d) *J. Am. Chem. Soc.* **2016**, *138*, 14202; (e) *Adv. Funct. Mater.* **2016**, *26*, 2435; (f) *ACS Energy Lett.* **2018**, *3*, 428; (g) *Inorg. Chem.* **2017**, *56*, 2596; (h) *J. Phys. Chem. Lett.* **2014**, *5*, 279; (i) *Chem. Mater.* **2014**, *26*, 6160.