

Tuning of band gap of colloidal organolead bromide perovskite nanocrystals by varying the size of the organic cation

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A few approaches have been employed to tune the band gap of colloidal organic-inorganic trihalide perovskites (OTPs) nanocrystals by changing the halide anion. However, to date there is no report of electronic structure tuning of perovskite nanocrystals upon changing the organic cation. For the first time, we have reported the non-template colloidal synthesis of bright green fluorescent $\text{CH}_3\text{NH}_3\text{PbBr}_3$ nanocrystals (NCs) with high quantum yield using ligand assisted reprecipitation technique (LARP) at room temperature. We have also tuned the band gap of $\text{CH}_3\text{NH}_3\text{PbBr}_3$ NCs by inserting the ethyl ammonium (EA) cation and varying the ratio of ethyl ammonium (EA) and methyl ammonium (MA) cations. It resulted into the formation of $(\text{EA})_x(\text{MA})_{1-x}\text{PbBr}_3$ NCs (where, x varies between 0 and 1) with band gap in the ranges 2.38 eV to 2.94 eV. The tuning of band gap is confirmed by electronic structure calculations within density functional theory which explain the increase in the band gap upon going towards larger 'A' site cations in APbBr_3 NCs. The photoluminescence quantum yield (PLQY) of these NCs lies between 5% to 85% and the average life-time falls in the range 1.4 ns to 215 ns.