

Origin of stability of all inorganic cesium lead halide perovskite nanocrystals: Surface ligand transition

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All inorganic cesium lead halide perovskite (CsPbX_3 , X is Cl, Br, or I) nanocrystals (NCs) prepared in solution have obtained immense attention because of their exceptionally high photoluminescence quantum yield, widely tunable emission colors, and dynamic interactions between surface atoms and organic ligands (surface–ligand interactions). Previously, instability of CsPbX_3 NCs was reported in several studies, and the dynamic surface–ligand interactions are postulated to induce such instability. In our previous study, we demonstrate stabilization of CsPbX_3 NCs by adding additional metal halides during the synthesis of NCs, and the enhanced stability was tentatively attributed to inorganically modified surfaces. Herein, we further reveal the origin of superstability of CsPbX_3 NCs. Various experimental characterizations (XPS, NMR, and TEM) and theoretical computational studies clearly demonstrate the origin of strikingly enhanced stability of the NCs in context of modified surface–ligand interactions.