Between molecules and nanocrystals: synthesis and properties of perovskite nanoclusters

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As a nanomaterial becomes smaller and smaller, bonds vibrate, quantum effects emerge and bulk effects become negligible: nanocrystals start to behave more like molecules and less like crystals. However, it is not yet clearly understood how molecular effects such as atomic vibrations and distortions affect ultrasmall clusters.

In this work, we investigate the transition between lead bromide complexes (i.e. $PbBr_6^{4-}$) and perovskite quantum dots. By using highly stable lead-ligand complexes as precursor, we were able to isolate monodisperse 1.2 nm, 1.8 nm, and 2.4 nm perovskite nanocubes. We investigate their optical and structural properties and demonstrate that the transition between multinuclear complexes and nanocrystals lies between cubes containing a total of 8 Pb atoms and cubes containing 27 Pb atoms. With temperature studies we determined that molecular distortions were the primary source of non-radiative recombination for smaller clusters and not surface defects. We expect our results to tremendously help understanding the fundamental properties of lead halide perovskite nanomaterials and their limitations as light-emitters.