

Disorder in cesium lead halide nanocrystals

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Cesium lead halide CsPbX₃ (X = Cl, Br, I) perovskite semiconductor nanocrystals (NCs) increasingly mesmerize researchers because they exhibit outstanding optoelectronic properties. One of the remaining hurdles is an atomistic structure determination due to their soft structure and their small size. We addressed this challenge by using nuclear magnetic resonance (NMR) spectroscopy.¹ This accessible technique can not only give insights into the elemental composition, but also into structural properties without having to manipulate or even damaging the labile samples during the measurements. The NC cores of colloidal solutions of perovskite semiconductor NCs could be studied in depth with solution NMR for the first time. The determination of surface and core sites could be done by probing various size selected NCs with an edge length between 3 and 12 nm. In doing so, a correlation between the chemical shift and the band gap of the NCs was observed, which was already predicted by theory. Furthermore, the distortions of the core structure induced by the dissimilar monodentate and zwitterionic capping ligands was studied, quantified, and could be correlated with their optical properties. *Ab initio* molecular dynamics simulations performed on various sizes of CsPbBr₃ NCs confirmed our observations. In mixed halide CsPb(Br/Cl)₃ NCs, an anion gradient was observed for the first time. These findings showcase the great potential of solution NMR in shedding light on the structure of colloidal semiconductor NCs.

[1] L. Piveteau, V. Morad, M.V. Kovalenko, *J. Am. Chem. Soc.* **2020**, 142, 46, 19413-19437.