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Planar Defects and morphology of CdSe QDs by SAXS/WAXS Total Scattering: Wurtzite versus Zincblende structure

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CdSe quantum dots (QDs) have been extensively studied in the last three decades because of their finely size- and shape- tunable optical and electronic properties. Its colloidal synthesis reached an advanced level of control over size and morphology, and fine engineering of the surface structure. Despite this, the fine control over nanocrystal defectiveness and the fundamental investigation of the surface structure and faceting still remains a highly challenging task that lacks established analytical approaches. We previously tackled this problem by combining X-ray total scattering techniques in the wide- (WAXS) and small-angle regions (SAXS) and using the Debye scattering equation (DSE) based modeling approach[1] to achieve a detailed characterization of size, morphology, and planar defects in oleate-capped zincblende CdSe QDs[2]. This DSE-based combined SAXS/WAXS method is now extended to the atomic-to-nanometer scale characterization of wurtzite ODPA-capped CdSe QDs in the 2.3 to 5.6 nm size range. The The NCs morphology is described as hexagonal truncated bipyramids, exposing {001}, {100} and {011} facets. The relative extension of the different facets was found being both size- and fault- dependent. The same atomistic models were simultaneously employed to model the WAXS region, where the presence of planar defects was introduced using a layer-by-layer approach in the model construction. The analysis indicated a radically different behavior of the planar defect concentration with comparison to the cubic CdSe QDs and extended results will be presented. This work shows the potential of the proposed analytical approach to untangle complex and intertwined features of crystal structure defectiveness and particles' morphology, which might have an important impact on the final properties of CdSe and semiconductors QDs in general.

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