MS38 Nanomaterials & graphene

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MS38-O1 Shape, Chemical and Crystalline Structure of Nanocrystals and their Impact on the Supercrystal Structure of Colloidal Superlattices

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The chemical synthesis of nanocrystals (NCs) has led to a pronounced improvement in the optical properties and the chemical stability of semiconducting NCs [1]. The optical emission of NCs can be drastically increased by stabilising the core with a hard protective shell [1]. For the cationic exchange based shell growth of PbS/CdS NCs [2], we have recently shown that metastable crystal phases in the CdS shell influences significantly the photoluminescence (PL). This was only achieved by retrieving the chemical profile of NCs in sub-nanometer resolution by using anomalous small angle x-ray scattering (ASAXS) in combination with the analysis of powder diffraction data by wide angle x-ray scattering (WAXS) [2]. In a current synchrotron study we have investigated CdSe/CdS core/shell NCs by recording ASAXS and WAXS spectra. We revealed that the epitaxial core/shell structure depicts again a sharp chemical interface. With increasing core diameter, however, the CdSe/CdS NCs deviate significantly from a spherical shape. By means of a recently developed shape retrieval method [3], we could reveal an elliptical NC shape with pronounced surface facets for the largest core/shell series. In combination with the WAXS data we could relate this anisotropic shape to specific crystallographic directions.

The NC's shape can also significantly influence the super-crystal structure of colloidal superlattices [1], when the NCs are used as building blocks. This we have shown, when we investigated with in-situ synchrotron SAXS the template free self-assembly of colloidal supercrystals based on nearly monodisperse Bi NCs [4]. The retrieved 3D mean shape [3] of the Bi NCs looks like a strongly facetted oblate ellipsoid and can be related to the rhombohedral crystal structure of Bi. Many sharp Bragg peaks prove the formation of well-ordered supercrystals, but we want to reveal if this superlattice structure can be directly related to the NC shape. Thus, we used the derived shape as input for a modeling of the crystallization process based on molecular dynamic simulations. Simulations and experiments show a good agreement and thus we are able to link the supercrystal structure via the NC-shape to the atomic Bi crystal structure.

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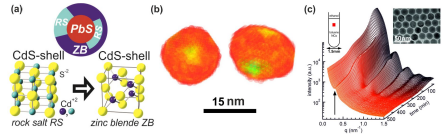

Figure 1. (a) Crystalline core/shell structure of PbS/CdS NCs derived by WAXS [3]. (b) From SAXS data derived elliptical and faceted shape of CdSe/CdS NCs. (c) *In-situ* SAXS study of the 3D self-assembly of colloidal supercrystals using Bi-NCs (see inset TEM) as building blocks.

Keywords: core/shell nanocrystals, colloidal supercrystals, synchrotron SAXS/WAXS