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Structural Profiles of Nanocrystals from ASAXS and Crystallographic Techniques

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The chemical synthesis of core/shell colloidal nanocrystals (NCs) have lead to an pronounced improvement in the optical properties and the chemical stability of semiconducting NCs [1]. The main topic of this work is the structural characterisation of core/shell NCs with anomalous small angle x-ray scattering (ASAXS) in combination with diffraction techniques (XRD) at laboratory- and synchrotron sources (HZB-BESSY and ESRF). Furthermore we complete these findings with complementary microscopy techniques (TEM). The detailed knowledge of the structural properties of the core/shell NCs allows to study the impact of the nanometer sized dimensions on their optical properties. The infrared emission of lead chalcogenide nanocrystals (NCs) in the size range of 5 - 10 nm can be drastically increased stabilising the core with a hard protective shell [1,2]., e.g., PbS/CdS NCs shows a higher efficiency and stability [2] with respect to pure PbS-NCs. In contrast to a shell growth on top of a core, we investigated in this study the CdS-shell growth on PbS NCs driven by Cd for Pb cation exchange [2]. Especially, we studied three different final shell thicknesses of 0.9, 1.5 and 2 nm. The chemical composition profile of the CdS-shell as a function of reaction time are derived from ASAXS experiments in sub-nanomter resolution. The crystal structure of the shell was derived by XRD combined with TEM measurements, respectively. We relate the chemical and structural information to the measured PL intensities of the core/shell NCs. We reveal the existence of two different crystalline phases, i.e. the metastable rock salt and the equilibrium zinc blende phase within the chemically pure CdS-shell. The highest improvement in the PL emission was achieved for 0.9 nm shells depicting a large metastable rock salt phase fraction matching the crystal structure of the PbS core. These results could be only achieved using ASAXS that gieves a mean chemical profile of a large ensemble of single core/shell NCs, but in sub-nanometer resolution [3].

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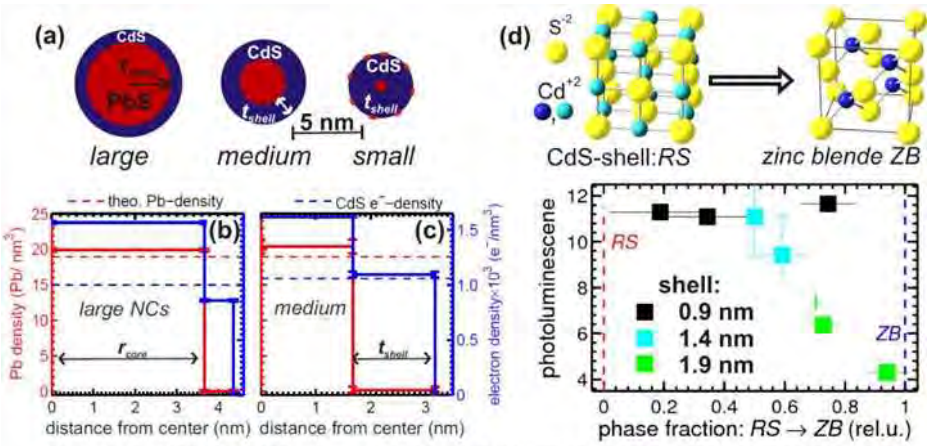

Figure 1: (a) Sketch of the investigated PbS/CdS core/shell NCs with three different sizes. (b) - (c) Chemical profiles of the large and medium sized NCs derived from ASAXS. (d) PL intenisty of the core/shell NCs as a function of the shell's crystal structure. The PL is normalised to the shell thickness as well to the total Pb amount within the NCs.

Keywords: Nanocrystal, ASAXS, crystal structure