Colloidal Nanocrystals: Relation between Structure and Functionality investigated by X-ray Scattering

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Chemical synthesised colloidal nanocrystals (NCs) offer the opportunity for realising novel materials with tailored functionalities. A large variety of semiconducting and metallic NCs can be realised[1]. Especially an inner core/shell structure of the semiconducting NCs leads to an increased photoluminescence (PL) output[1-3]. But also the NCs' shape determines their optical performance. We have revealed a relation between structure and functionality by combining different scattering techniques at lab and synchrotron sources with microscopy techniques[2,3]. In a study at the synchrotron ESRF, we have investigated hexagonal CdSe/CdS core/shell NCs with different dimensions by recording ASAXS and WAXS spectra. By means of a 3D shape retrieval method for SAXS data[4,5], we could reveal an elliptical particle shape with pronounced surface facets for the largest core/shell NCs and related this shape to specific crystallographic directions. The increased anisotropy is directly connected to a decreased PL.

The NC's shape can also significantly influence the super-crystal structure of colloidal supercrystals[1], where NCs act as building blocks to form 3D nanocrystal solids with designed properties. We were able to link their supercrystal structure to the atomic Bi NC structure[5].

References:

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