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. 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]. In a recent 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 shape retrieval method for SAXS data [3, 4], 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 [4].