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. 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. 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, 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, 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.

References: