

MS40-P13 | INTERPLAY BETWEEN CRYSTAL STRUCTURE, SHAPE AND FUNCTIONALITY OF COLLOIDAL NANOCRYSTALS AND SUPERCRYSTALS

Lechner, Rainer T. (Montanuniversitaet Leoben, Leoben, AUT); Ludescher, Lukas (Montanuniversitaet Leoben, Leoben, AUT); Burian, Max (TU Graz, Graz, AUT); Karner, Carina (University of Vienna, Wien, AUT); Amenitsch, Heinz (TU Graz, Graz, AUT); Yarema, Maksym (ETH Zurich, Zürich, CH); Dirin, Dmitry N. (ETH Zurich, Zürich, CH); Kovalenko, Maksym V. (ETH Zurich, Zürich, CH); Heiss, Wolfgang (FAU Nürnberg Erlangen, Nürnberg, GER); Dellago, Christoph (University of Vienna, Wien, AUT)

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].

[1] M. V. Kovalenko, et al., & W. Heiss, *ACS Nano* 9, 1012–1057 (2015)

[2] L. Ludescher, et al., & R.T. Lechner, *Front. Chem.* 6, 672 (2019)

[3] M. Burian, G. Fritz-Popovski, et al., & R.T. Lechner, *J. Appl. Cryst.* 48, 857-868 (2015)

[4] M. Burian, C. Karner, et al., & R.T. Lechner, *Adv. Mater.* 30, 1802078 (2018)