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Multiple scale characterisation of ultrasmall nanocrystals by X-ray Total Scattering

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Fundamental aspects and an overview of applications of cutting-edge nanocrystallography tools grounded on Wide Angle X-ray Total Scattering (WAXTS) techniques (mainly synchrotron-based) and the use of the Debye Scattering Equation (DSE) for data modeling in reciprocal space will be presented. [1,2]
The approach overcome the limits of conventional diffraction-based methods for characterizing engineered ultrasmall nanocrystals and, by exploiting the full (Bragg and diffuse scattering) information in the experimental data, is able to quantitatively recover atomic and nanometer scales properties (structural distortions, defects of various kind, lattice strains, surface relaxation, size, morphology and their relative dispersion) suitably encoded in the same atomistic model. Combining WAXTS with Small Angle X-ray scattering (SAXS) data fruitfully exploits their complementarity for a more robust, quantitative multiple-scale analysis and/or for disentangling size/shape from structural defects-induced effects.

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