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Impact of ethylenediaminetetraacetate ligands on CdS nanoparticle formation mechanism

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Organic ligands are commonly employed to stabilize nanoparticle sizes, shapes and long-term colloidal stability in dispersions. For Cadmium chalcogenides, ethylenediaminetetraacetate (EDTA) seems a good candidate due to its strong chelating action towards Cd^{2+} . Further, EDTA-capped CdS nanoparticles were proven to be stable in aqueous dispersion at room temperature over months.[1,2]

Without ligands, the CdS nanoparticles nucleate via a two-step formation mechanism involving $\text{Cd}_{13}\text{S}_4(\text{SH})_{18}$ precursor particles and a diffusion-driven growth process to ca. 5 nm particles within 2.5 ms.[3] Yet, up to now no mechanistic insight into the CdS particle formation in presence of EDTA has been provided.

Here we evidence the formation of ca. 5 nm sized EDTA-capped CdS particles from $\text{CdCl}_2/\text{EDTA}$ and Na_2S stock solutions with SANS and laboratory SAXS. The mixing speed and / or solvent (H_2O / D_2O) seem to impact the particle diameter. Contrast matching in SANS not only accesses the ligand shell, but also reveals an unexpected superstructure formation on a time scale of hours. pH-dependent studies and multinuclear and multidimensional solid-state NMR spectroscopy complement insight into the EDTA binding.[4]

[1] G. H. Reed, et al, Inorg. Chem. 1971, 10

[2] A. A. Rempel, et al, Russ. Chem. Bull. 2013, 62, 398

[3] A. Schiener, et al, Nanoscale 2015, 7, 11328

[4] S. W. Krauss, et al, in preparation

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