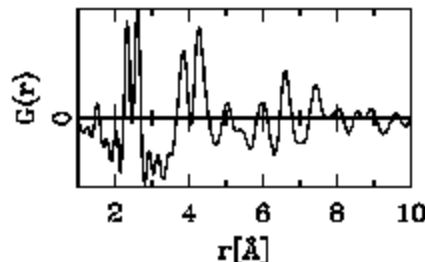


Structure of CdSe/ZnS Core/Shell Nanoparticles. R.B. Neder, Institut fuer Mineralogie, Univ. Wuerzburg, Am Hubland, 97074 Wuerzburg, Germany.

The structure of CdSe/ZnS core/shell nanoparticles was determined from pair distribution function(PDF), small angle X-ray scattering, standard and anomalous powder diffraction, and EXFAS data. The particles were prepared as described by [1]. The powder pattern reveal broad maxima that indicate a zinblende structure and particles with approximately 3 to 4 nm in diameter.



Both, EXAFS and PDF data reveal that the first neighbour distances Cd-Se (2.61) and Zn-S (2.33) correspond to their respective bulk values. The PDF data furthermore show that also the next few neighbour distances are identical to the respective bulk values as well. The width of the first neighbour distributions is not wider than that of standard reference samples.

This proves that the CdSe core and the ZnS shell are free of substantial strain. The thin ZnS shell is thus not epitaxially grown with pseudomorphic lattice constants but has already relaxed to the bulk structure. The complementary combination of the experimental data enabled to determine and refine a full structural model.

[1] Dabbousi, B. O., Rodriguez-Viejo, J., Mikulec, F. V., Heine, J.R., Mattoussi, H., Ober, R., Jensen, K. F. & Bawendi, M. G. J. Phys. Chem. B, 101, 9463 (1997).