Dopant Position in Inorganic Semiconductor Nanoparticles from Reverse Monte Carlo (RMC) analysis of Extended X-ray Absorption Fine Structure (EXAFS) Spectra

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Typical semiconductor dopant concentrations imply that most nanoscaled particles in an ensemble are undoped and the doping level for particles actually containing dopant atoms is orders of magnitude higher compared to the bulk level. Hence, doping of semiconducting nanoparticles has a completely different character compared to bulk systems. In order for the dopant atom to be electrically functional – to provide mobile charge carriers – it should form shallow impurity levels in the host semiconductor. Deep impurity centers typically generate a larger (local) distortion of the host lattice and trap charge carriers. Therefore, the challenge is, to control and determine the distribution of the dopant atoms relative to the particle surface and the location of the dopant atoms relative to the crystal lattice. Extended X-ray Absorption Fine Structure (EXAFS) and X-ray Absorption Near Edge Structure (XANES) in X-ray absorption spectra contain the relevant element-specific information of the local structure.

We found in silver doped cadmium selenide that even a few Ag atoms can potentially enhance the fluorescence of the CdSe nanocrystals dramatically [1]. In this contribution we report a detailed investigation about the sites on which the dopant atoms are located from K-edge XAFS spectra measured for all three elements, namely Cd, Se, and Ag [2]. Extensive analysis of the local structure of CdSe nanocrystals doped with Ag by ion exchange shows that Ag is located on (distorted) tetrahedral interstitial sites either in a wurtzite or zinc blende lattice, the local structure around Ag being similar to Ag_2Se. The local structure does not depend on the dopant content between 0 and 2.5% Ag. Indirect evidence has been obtained that Ag is not located at the particle surface but incorporated into the nanocrystal.

References

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[2] A. Kompch, A. Sahu, Chr. Notthoff, F. Ott, D. J. Norris, and M. Winterer, *Localization of Ag Dopant Atoms in CdSe Nanocrystals by Reverse Monte Carlo Analysis of EXAFS Spectra,* J. Phys. Chem. C **119** (2015), 18762.

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