Atomistic Modelling of CdSe/CdS Dotrods (DR)

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CdSe/CdS DRs have interesting optical properties. They have a high photoluminescence quantum yield while showing almost no blinking behavior. Additionally the emitted light is linear polarized. The synthesis of DRs is done by using a hot injection reaction to grow an elongated CdS shell around the spherical CdSe core forming a single nanocrystal (with wurtzite crystal structure). Due to the difference in lattice parameters the interface between the core and the shell is strained, which primarily leads to a compression of the core and distortion of the shell.

We have developed an atomistic model to estimate the strain profile in those DR. Therefore we built model structures of DR with defined symmetry. By applying a Keating valence force field the bond angles and lengths can be relaxed to minimize the strain energy.[1] Figure 1 shows how the bond lengths inside a 20 nm-5 nm-4 nm-(shell length–shell diameter–core diameter)-DR change compared to bulk bond lengths. The calculated data fits nicely to other models shown in literature.[2] We observe interesting effects when systematically changing different parameters. Smaller cores and thicker shells increase the strain on the core. If the shell is thin compared to the core there are only few layers of atoms enclosing the core at the thinnest spot and these atoms undergo heavy distortion. The length of the shell is proven to have no further influence on the core once a certain length is reached.

The obtained theoretical data can be compared to measurements of the flourescence spectra and the polarisation anisotropy to correlate the strain to the optical properties. The control of the shell diameter was previously not possible without also influencing the length of the shell, but is now synthetically accessible.[3] This allows to synthesize CdSe/CdS DR with tailor-made properties.

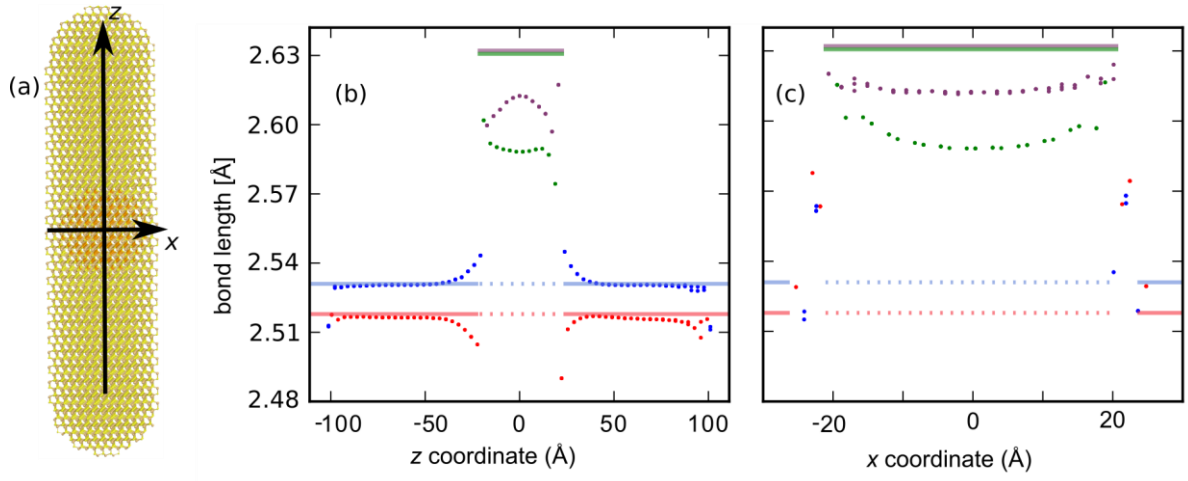

Fig. 1 (a) Atomistic model of a DR with a length of 20 nm, a diameter of 5 nm and a core diameter of 4 nm. (b, c) Calculated bond lengths for positions along (b) the *z* coordinate (long direction of the DR) and (c) the *x* coordinate (along the diameter of the DR). Here, the colorcode accounts for different bond types in the crystal. red: Cd-S-bonds along *z*, blue: Cd-S-bonds along *x*, purple: Cd-Se-bonds along *z*, green: Cd-S-bonds along *x*.

1) D. Camacho *et al.*, *Physica E*, **2010**, *42*, 1391-1364.
2) Y. Luo *et al.*, *ACS Nano*, **2010**, *4*, 91-98.
3) I. Coropceanu *et al.*, *ACS Nano*, **2016**, *10*, 3295–3301.