Quantification of Material Gradients in Nanocrystals[1]

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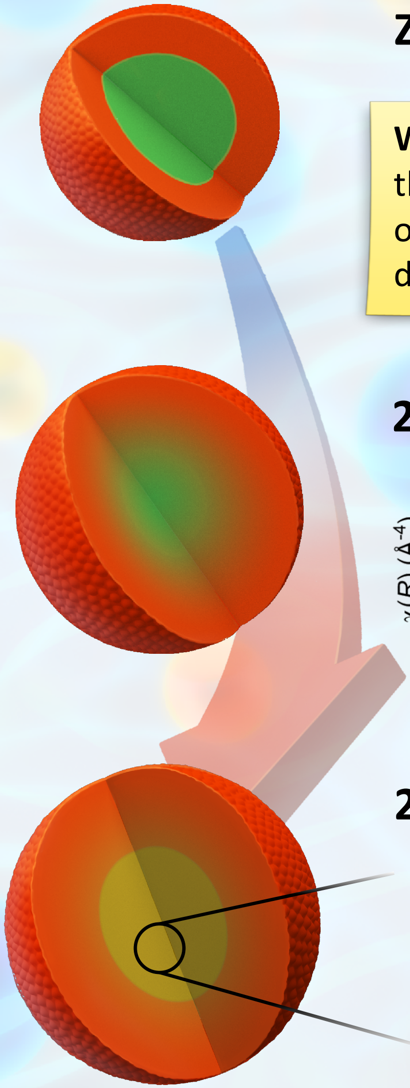


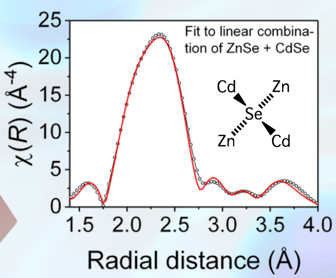
ZnSe/CdS: Type-II structure with temperature-induced gradients

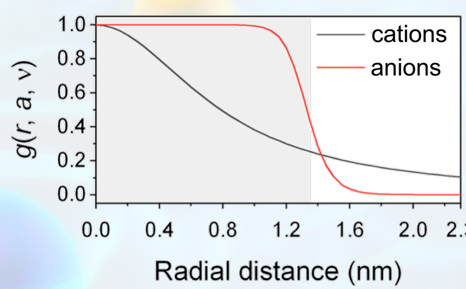
What? Quantification of the interfacial gradient of core/shell semiconductor nanocrystals.

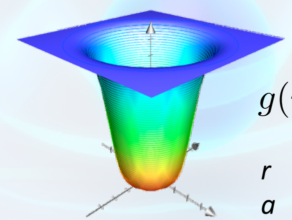
Why? Gradients improve optical properties,[2] but knowledge on their structure is lacking.

How? Fit of a gradient model[3] to the average coordination from a Se K-edge EXAFS spectrum.

260 °C: Strong cation diffusion already at typical shell growth conditions



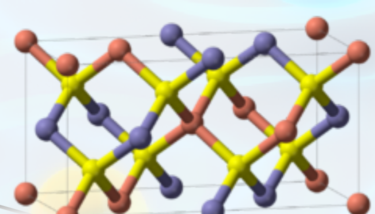


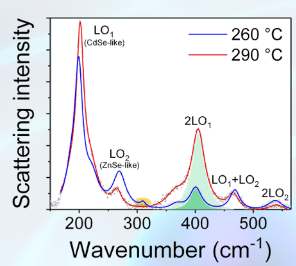


$$g(r, a, \nu) = \frac{r^\nu}{r^\nu + a^\nu}$$

r distance from centre
a point of inflection
ν gradient slope

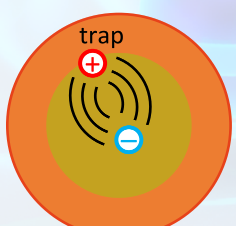
290 °C: An ordered $Zn_{0.5}Cd_{0.5}Se$ superlattice in the core minimises strain[4]





Raman Spectra (λ = 785 nm):

- Almost no CdS LO phonon
- Strongly enhanced $2LO_1$ overtone (290 °C sample)
- Sub band-gap resonant Raman scattering
- Exciton trapped at interface



[1] Boldt et al., *Nano Lett.* **2020**, *20*, 1009; [2] Boldt et al., *Chem. Mater.* **2013**, *25*, 4731; [3] Cragg et al., *Nano Lett.* **2010**, *10*, 313; [4] Wei et al. *Phys. Rev. B* **1990**, *41*, 8240.