hkl-based calculation of total scattering patterns from discrete structure models using TOPAS

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It is demonstrated how *TOPAS* [1] can be utilized for the discrete modelling of nanocrystals and the calculation of total scattering patterns [2]. The limitations of the conventional Rietveld method are overcome by placing the nanocrystal structure model (in space group P1) in a large otherwise empty supercell disrupting the periodicity and generating a large number of hkls. Figure 1 shows the number of hkls and scattering intensity increasing proportionally to the supercell volume and merging into the diffuse pattern. In combination with the thermal diffuse scattering the same results are obtained as with the Debye Scattering Equation [2, 3]. Respective structure models can be added to a *TOPAS* refinement like any other crystal structure and are suitable for quantitative analysis. The same models are also suited for the composite PDF modelling [4].

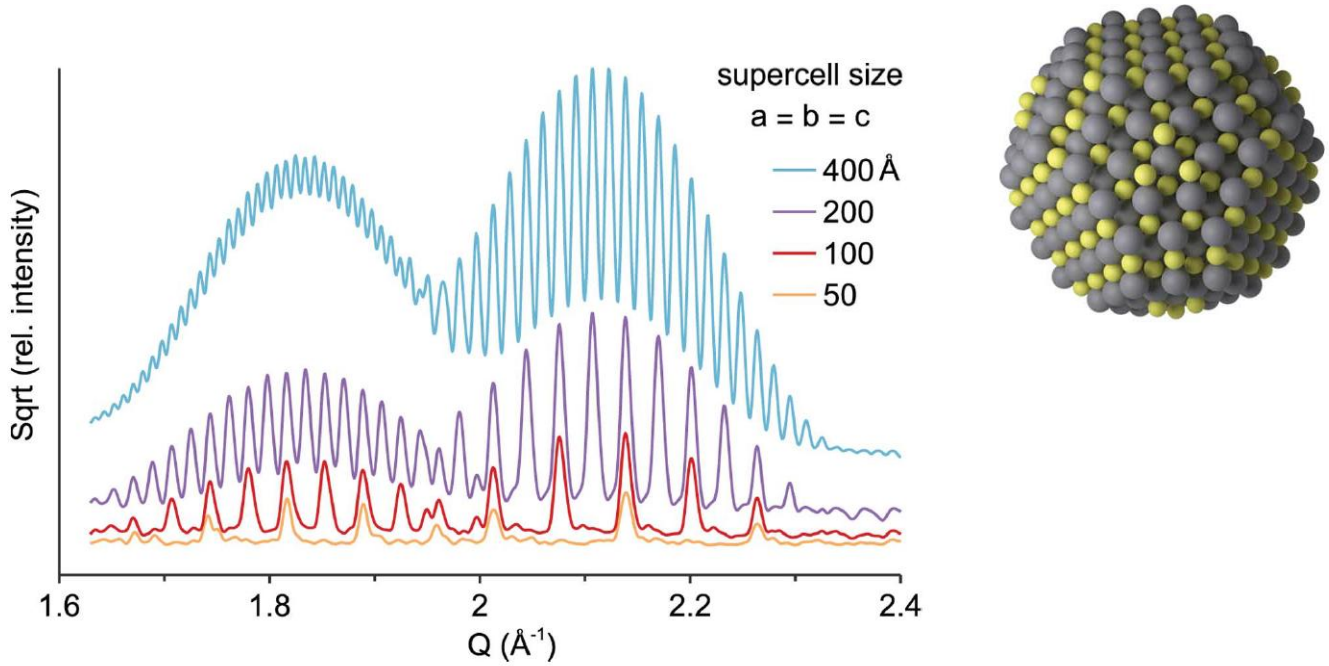


Figure 1. *Calculated pattern of a 3.5 nm PbS quantum dot [5] at increasing supercell size.*

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