Electronic supplementary data

Considerations on the model free shape retrieval of inorganic nanocrystals from SAXS data

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1. Overview

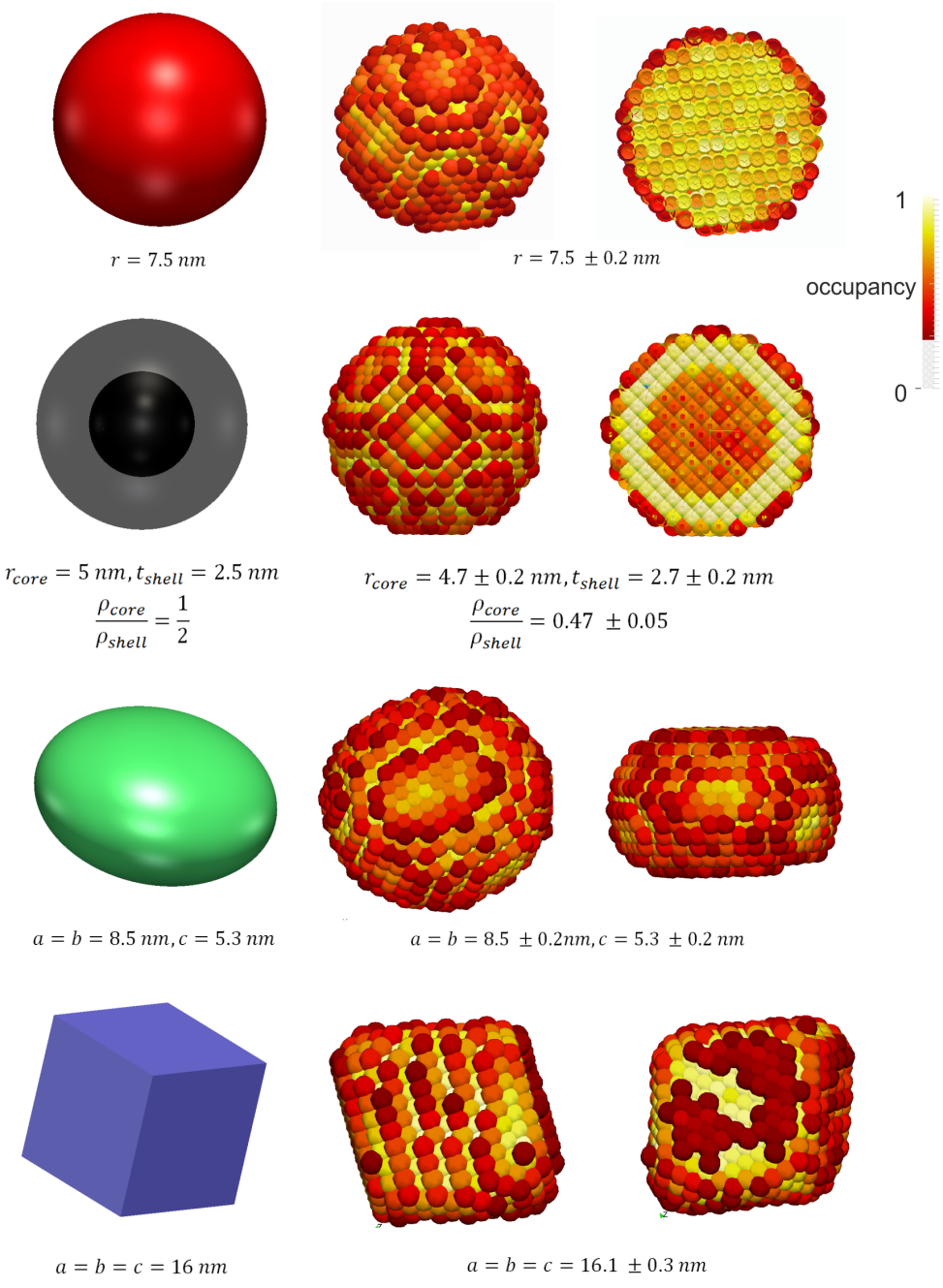

Fig. S1. Overview of the geometries presented in this work. The first left column shows the used initial shapes, the two rigth columns the retrieved aDAM shape models. The corresponding scattering curves can be found in Fig. S2-4. The values obtained using the aDAM evaluation methods presented in this work are shown using the suggested error with a magnitude of the dummy atom diameter.

2. Scattering Data

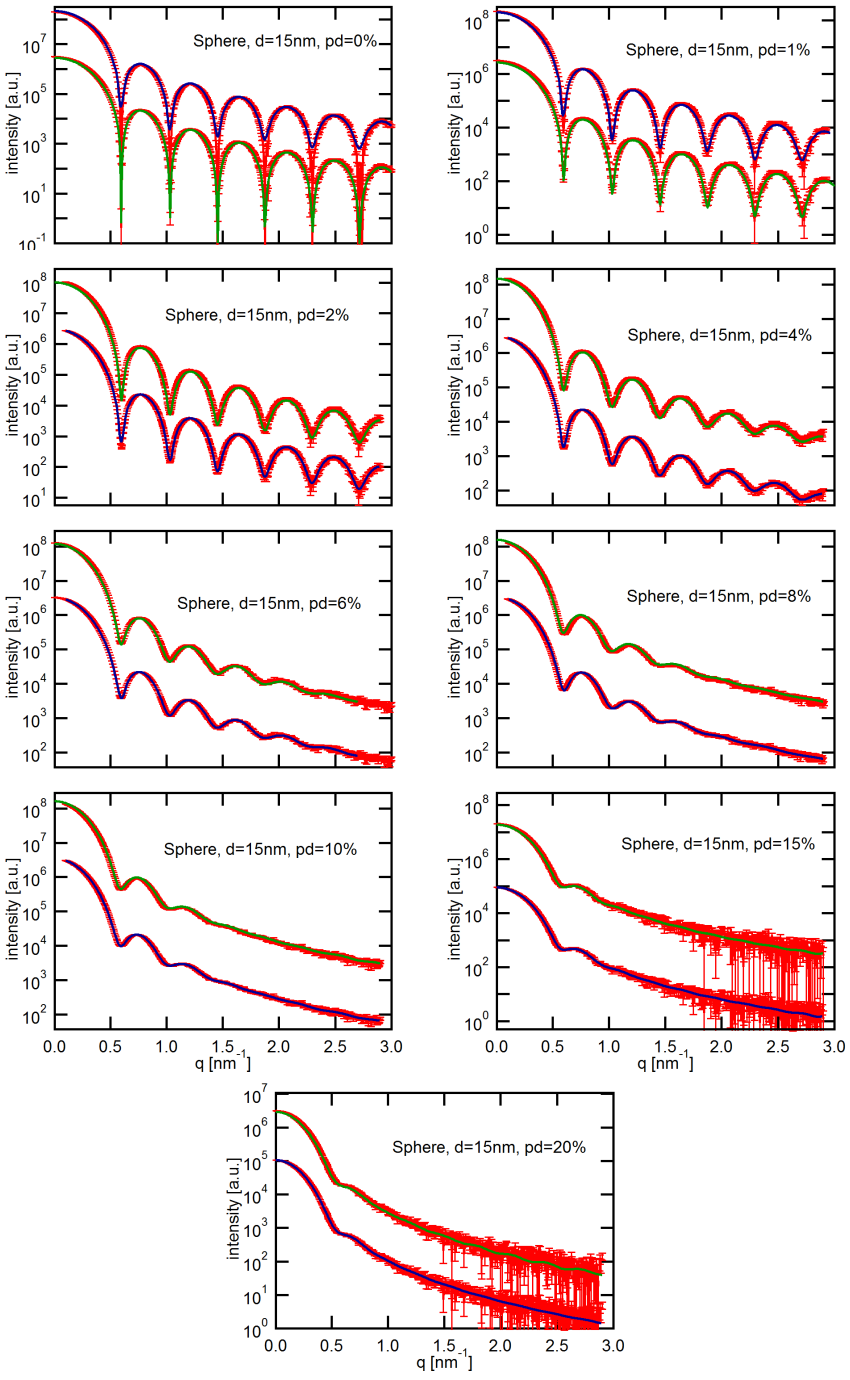

Fig. S2. Scattering data used for the computation of the aDAMs regarding the investigation of polydisperse spheres. The computed initial scattering curves (red), the p(r) obtained from GNOM (green) as well as the averaged DAMMIN fits (blue) are shown.

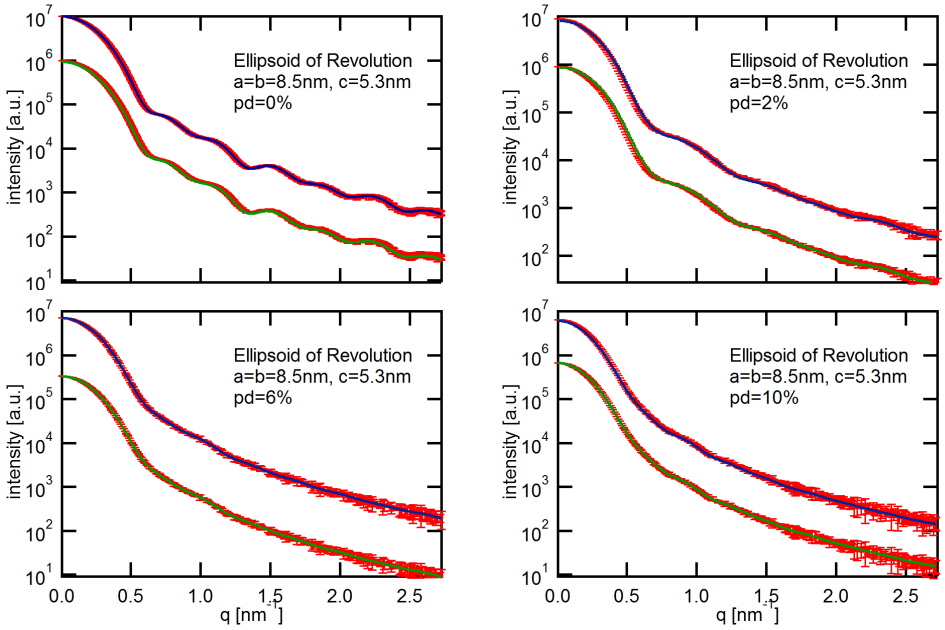

Fig. S3. Scattering data used for the computation of the aDAMs regarding the investigation of polydisperse ellipsoids of revolution. The computed initial scattering curves (red), the p(r) obtained from GNOM (green) as well as the averaged DAMMIN fits (blue) are shown.

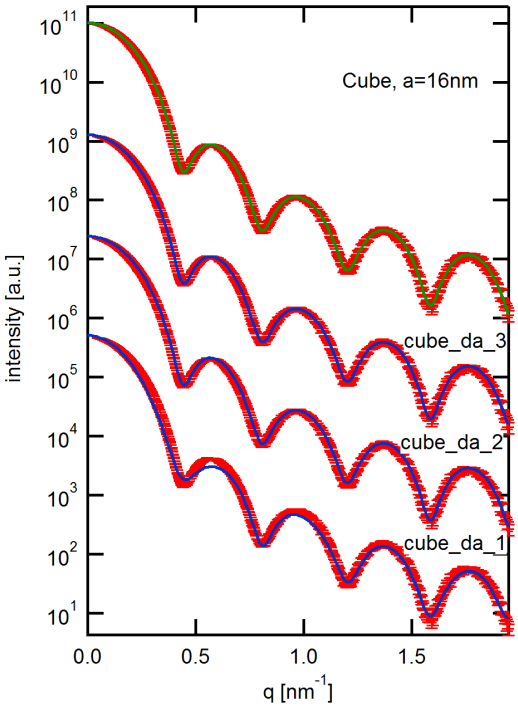

Fig. S4. Scattering data used for the computation of the aDAMs regarding the investigation of effects of decreasing numbers of DAs. The simulations cube_da_1, cube_da_2 and cube_da_3 correspond to 2988, 5594 and 8853 DAs in the initial search volume, respectively. The computed initial scattering curves (red), the p(r) obtained from GNOM (green) as well as the averaged DAMMIN fits (blue) are shown.

3. Normalized Spatial Discrepancy (NSD)

Table S1. *Average NSD values from the DAMAVER procedure of all averaged dummy atom models (aDAMs) shown in this work, whereas for every aDAM 10 independent dummy atom models (DAMs) were used. In the case of spheres and ellipsoids of revolution, σ represents the standarad deviation of the Gaussian size distributions used to smear the system. Also the effects of varying numbers of Shannon channels (SCs) and dummy atoms (DAs) are shown.*

sphere		ellipsoid		core shell		cube	
σ[%]	NSD	σ[%]	NSD	SCs	NSD	DA	NSD
0	0.493±0.003	0	0.490± 0.006	20	0.463±0.006	8853	0.444±0.010
1	0.481±0.002	2	0.441± 0.015	15	0.472±0.004	5594	0.443±0.007
2	0.460±0.004	6	0.449± 0.011	10	0.477±0.005	2988	0.540±0.010
4	0.474±0.020	10	0.452± 0.007	5	0.467±0.007		
6	0.460±0.011						
8	0.459±0.004						
10	0.457±0.005						
15	0.432±0.017						
20	0.499±0.015						

Table S2. *NSD values of averaged dummy atom models (aDAMs) from polydisperse model systems, compared to the aDAM retrieved for perfect monodispersity. The values were computed using SUPCOMB. σ represents the standarad deviation of the Gaussian size distributions used to smear the system.*

σ[%]	1	2	4	6	8	10	15	20
sphere	0.4493	0.4441	0.4584	0.4731	0.4814	0.5033	0.8095	0.8840
ellipsoid		0.4815		0.4960		0.6165		