

$\text{Na}_{1,5-\frac{x}{2}}\text{Sr}_x\text{Gd}_{1,5-\frac{x}{2}}\text{F}_6$ nanocrystals ($0 \leq x \leq 1$): Growth, size control
and shell formation on $\beta\text{-NaREF}_4$ core particles
Supporting Information

J. Wehmeier and Markus Haase

July 8, 2020

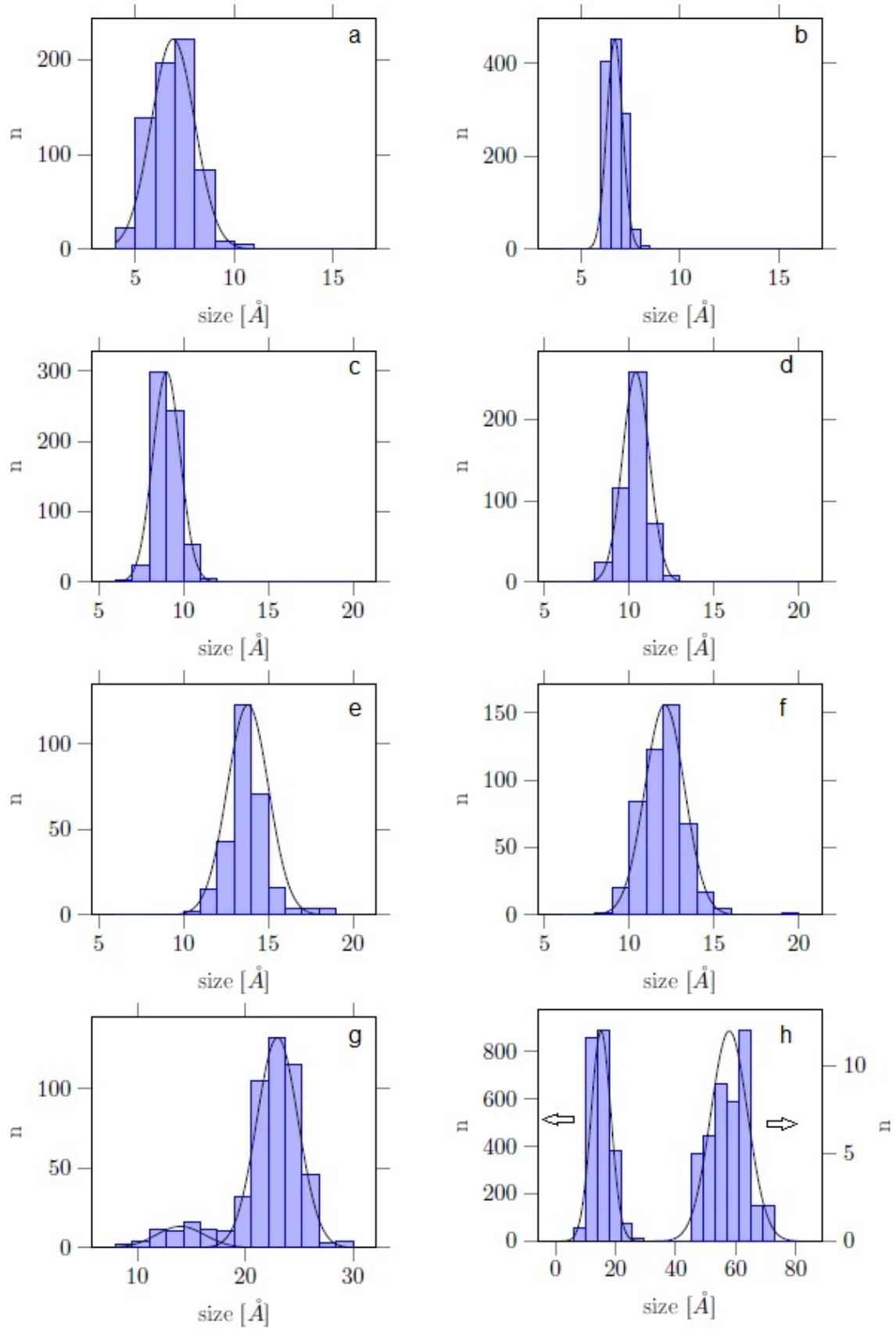


Figure S1: Particle size distribution of the $\text{Na}_{1.5-\frac{x}{2}}\text{Sr}_x\text{F}_{1.5-\frac{x}{2}}\text{F}_6$ -nanoparticles with (a) $x=0.2$, (b) $x=0.4$, (c) $x=0.5$, (d) $x=0.6$ (e) $x=0.7$ (f) $x=0.75$, (g) $x=0.8$ and (h) $x=1$.

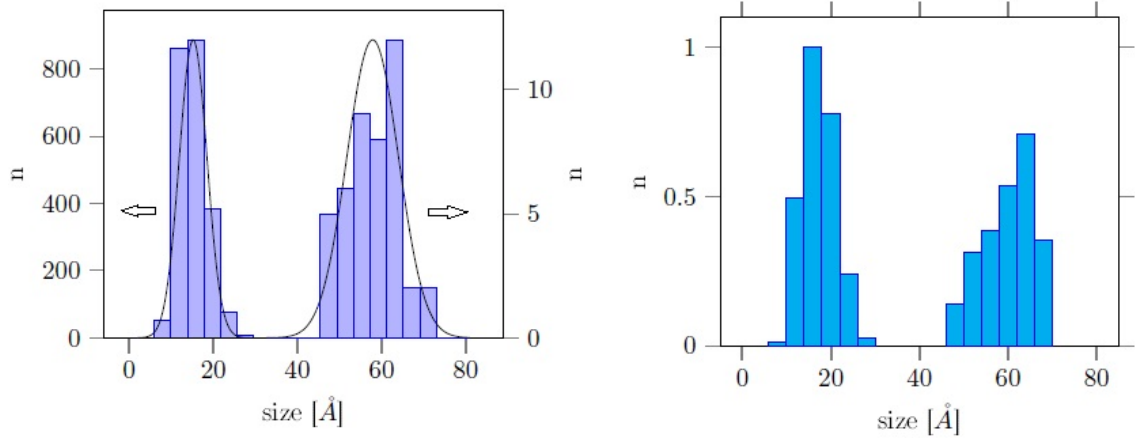


Figure S2: Particle size distribution of NaSrGdF_6 ($x=1$) particles weighted by the number of the particles (left) and weighted by volume of the particles (right).

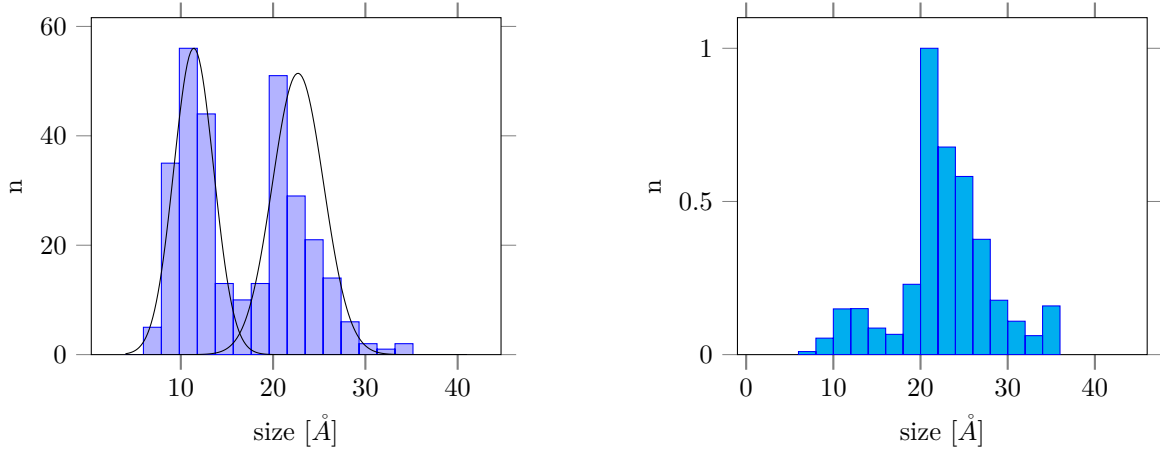


Figure S3: Particle size distribution of the $\beta\text{-NaSrGdF}_6@ \beta\text{-Na}_{1.125}\text{Gd}_{1.125}\text{Sr}_{0.75}\text{F}_6$ core/shell particles weighted by the number of the particles (left) and weighted by volume of the particles (right).

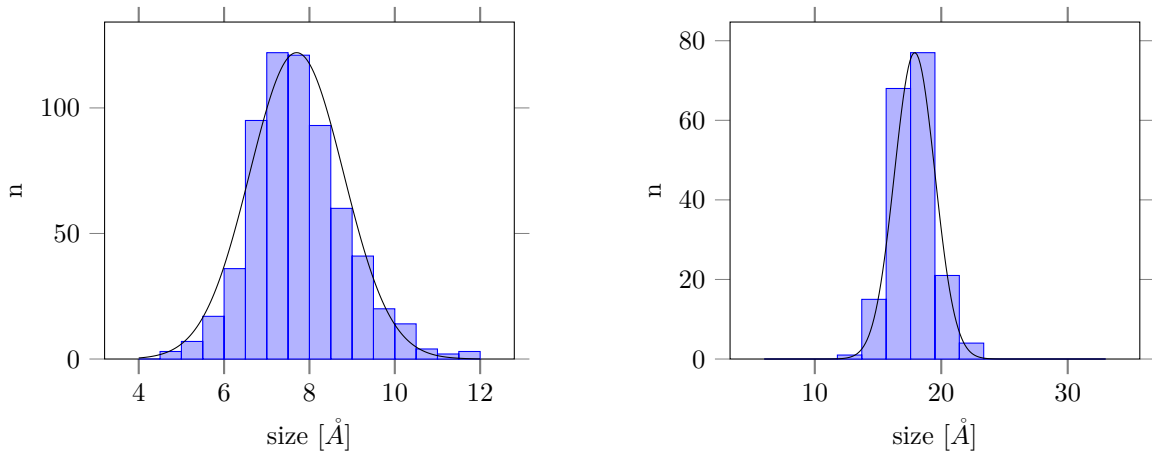


Figure S4: Particle size distribution of the $\beta\text{-NaCeF}_4$: 25%Tb core particles (lef) and $\beta\text{-NaSrGdF}_6@ \text{NaCeF}_4$: 25%Tb core/shell particles (right).

x	average size $\pm$ standard deviation [nm]	standard deviation [%]
0.2	6.9 $\pm$ 1.10	16.1
0.4	6.7 $\pm$ 0.40	6.0
0.5	10.4 $\pm$ 0.79	7.6
0.6	9.0 $\pm$ 0.81	9
0.7	13.8 $\pm$ 1.22	8.8
0.75	12.2 $\pm$ 1.17	9.6
0.8	23.1 $\pm$ 1.92	7.6
1	16 $\pm$ 2.9 (α -particles) 57 $\pm$ 5.5 (β -particles)	18.1 (α) 9.6(β)
0.97 (core/shell)	11.4 $\pm$ 2.16 (α) 22.7 $\pm$ 2.78 (β)	18.8 (α) 12.3(β)
NaCeF ₄ :Tb core	7.7 $\pm$ 1.06	13.8
NaCeF ₄ :Tb core/shell	17.8 $\pm$ 1.61	9.0

Table S1: Size distribution of the $\text{Na}_{1.5-\frac{x}{2}}\text{Sr}_x\text{Gd}_{1.5-\frac{x}{2}}\text{F}_6$ and core/shell nanoparticles, values of the mean size and the standard deviation as derived from TEM images.

x (synthesis)	equivalent molar ratio Sr/Gd (synthesis)	x (XRF)	equivalent molar ratio Na:Sr:Gd (XRF)
0.2	0.14:1	0.21	1.15:0.15:1
0.4	0.31:1	0.41	1.21:0.32:1
0.5	0.4:1	0.52	1.01:0.42:1
0.6	0.5:1	0.64	1.00:0.54:1
0.7	0.61:1	0.73	0.95:0.64:1
0.75	0.67:1	0.82	1.10:0.75:1
0.8	0.73:1	0.86	0.84:0.80:1
0.97	0.95:1	0.95	0.88:0.92:1

Table S2: Atomic composition of the $\text{Na}_{1.5-\frac{x}{2}}\text{Sr}_x\text{Gd}_{1.5-\frac{x}{2}}\text{F}_6$ -nanoparticles and the $\beta\text{-NaSrGdF}_6@ \beta\text{-Na}_{1.125}\text{Gd}_{1.125}\text{Sr}_{0.75}\text{F}_6$ core/shell particles, as determined by X-ray fluorescence analysis

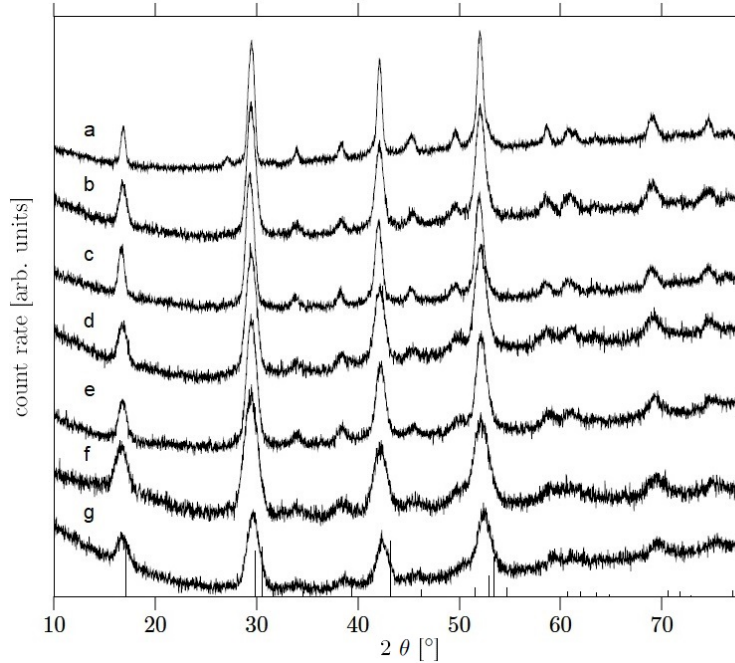


Figure S5: XRD data of the $\text{Na}_{1.5-\frac{x}{2}}\text{Sr}_x\text{Gd}_{1.5-\frac{x}{2}}\text{F}_6$ -nanoparticles with a) $x=0.8$, b) $x=0.75$, c) $x=0.7$, d) $x=0.6$, e) $x=0.5$, f) $x=0.4$ and g) $x=0.2$. Intensities are normalized.

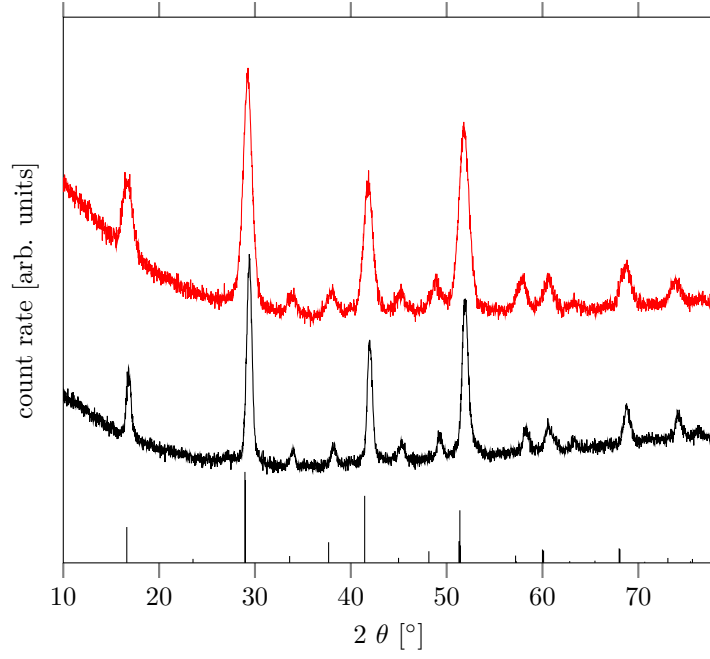


Figure S6: XRD data of β -NaCeF₄: 25%Tb core particles (red) and NaSrGdF₆@ β -NaCeF₄: 25%Tb core/shell particles (black). The vertical lines correspond to the reference pattern of β -NaCeF₄ (ICSD-# 31608).

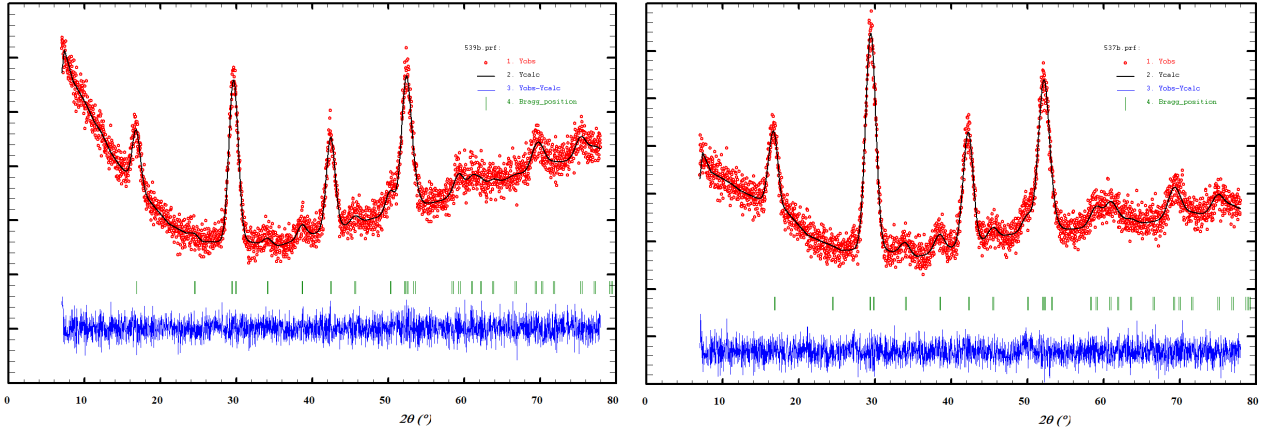


Figure S7: Rietveld fits of the XRD data of Na_{1.5-x/2}Sr_xGd_{1.5-x/2}F₆-nanoparticles with x=0.2 (left) and x=0.4 (right)

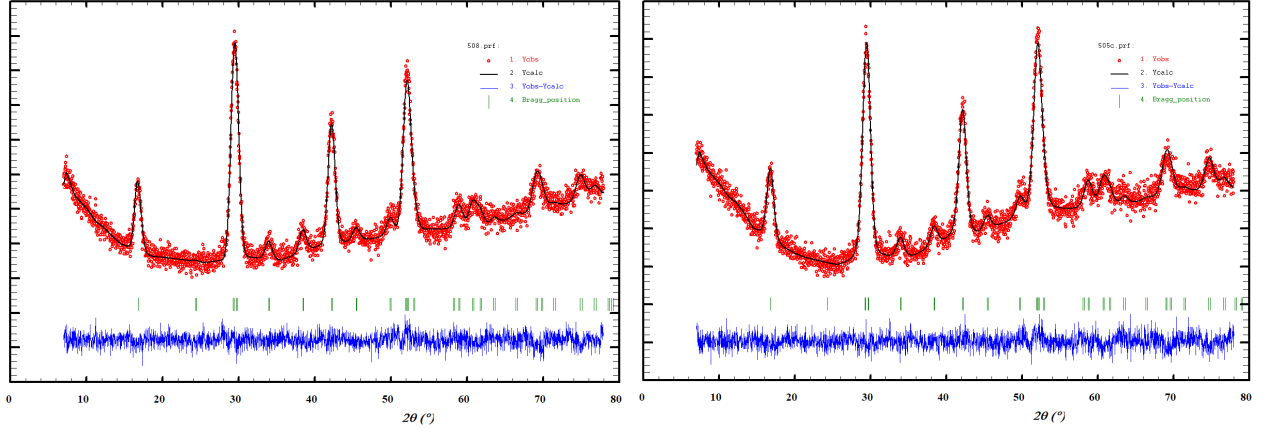


Figure S8: Rietveld fits of the XRD data of $\text{Na}_{1,5-\frac{x}{2}}\text{Sr}_x\text{Gd}_{1,5-\frac{x}{2}}\text{F}_6$ -nanoparticles with $x=0.5$ (left) and $x=0.6$ (right)

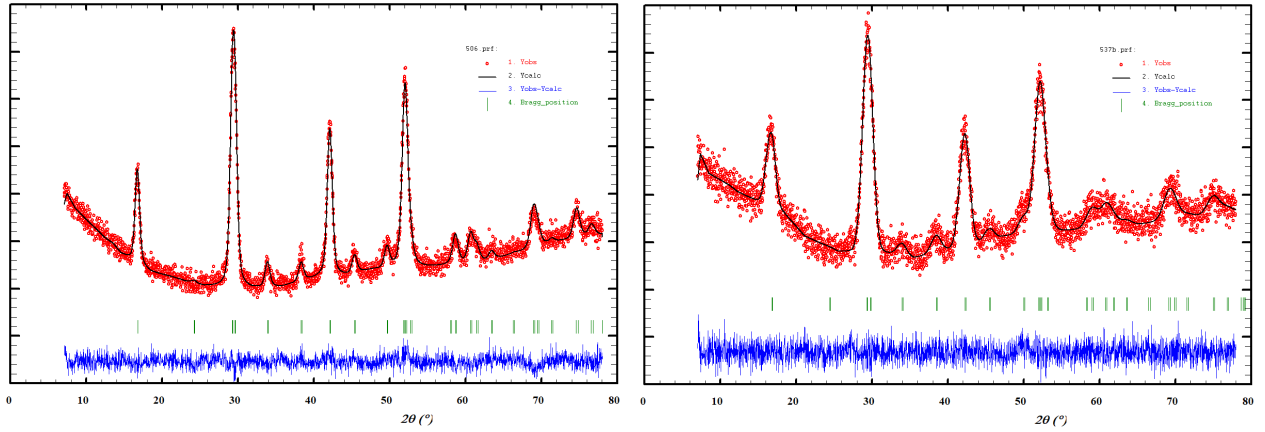


Figure S9: Rietveld fits of the XRD data of $\text{Na}_{1,5-\frac{x}{2}}\text{Sr}_x\text{Gd}_{1,5-\frac{x}{2}}\text{F}_6$ -nanoparticles with $x=0.7$ (left) and $x=0.75$ (right)

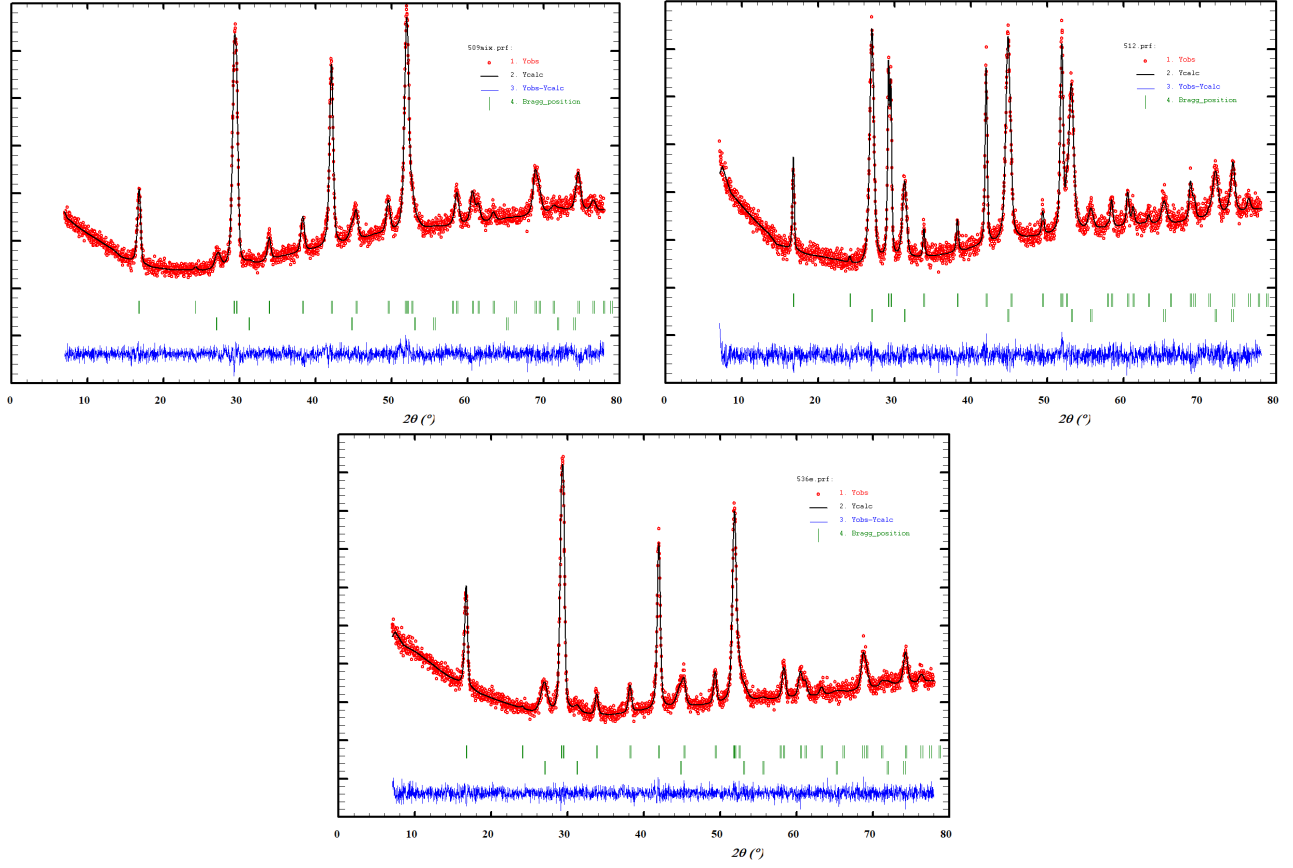


Figure S10: Rietveld fits of the XRD data of $\text{Na}_{1.5-x}\text{Sr}_x\text{Gd}_{1.5-x/2}\text{F}_6$ -nanoparticles with $x=0.8$ (top left), $x=1$ (top right), and the $\beta\text{-NaSrGdF}_6@ \beta\text{-Na}_{1.125}\text{Gd}_{1.125}\text{Sr}_{0.75}\text{F}_6$ particles (bottom)