Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Paramagnetic Electron Centers in $BaTiO_3$ Nanoparticle Powders

Ellie Neige, Oliver Diwald

Department of Chemistry and Physics of Materials,

Paris Lodron Universität Salzburg,

Jakob-Haringer Strasse 2a, A-5020 Salzburg (Austria) E-mail: oliver.diwald@sbg.ac.at

S1

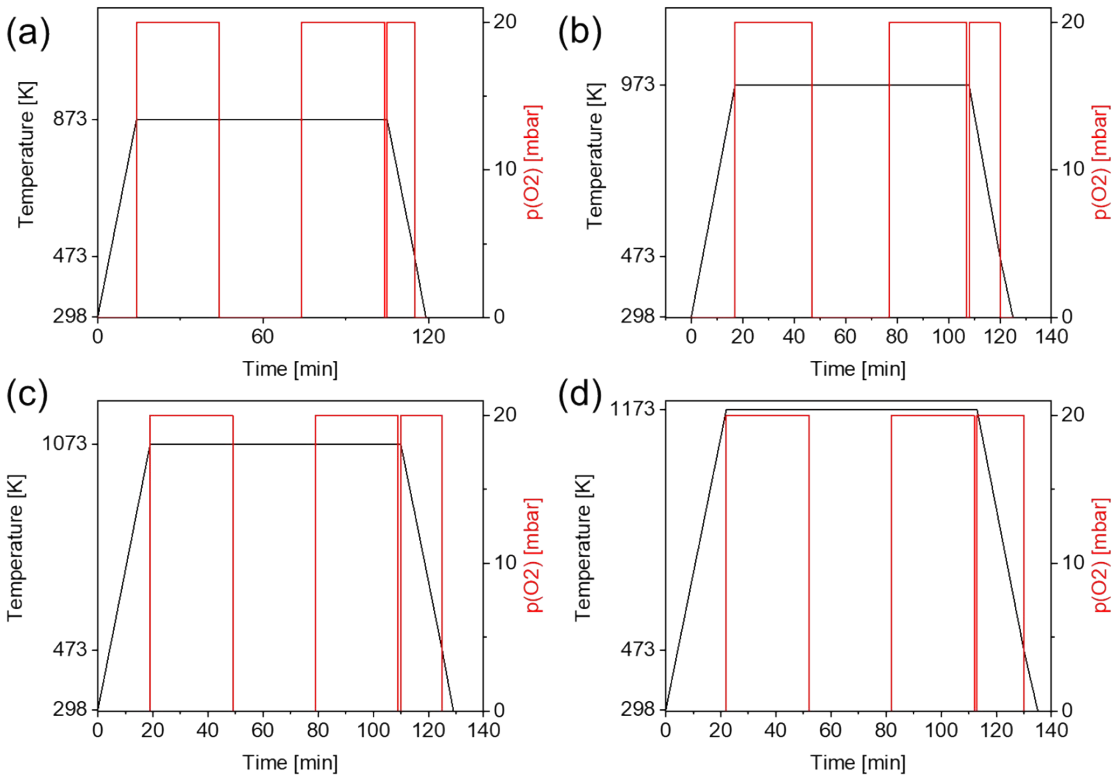
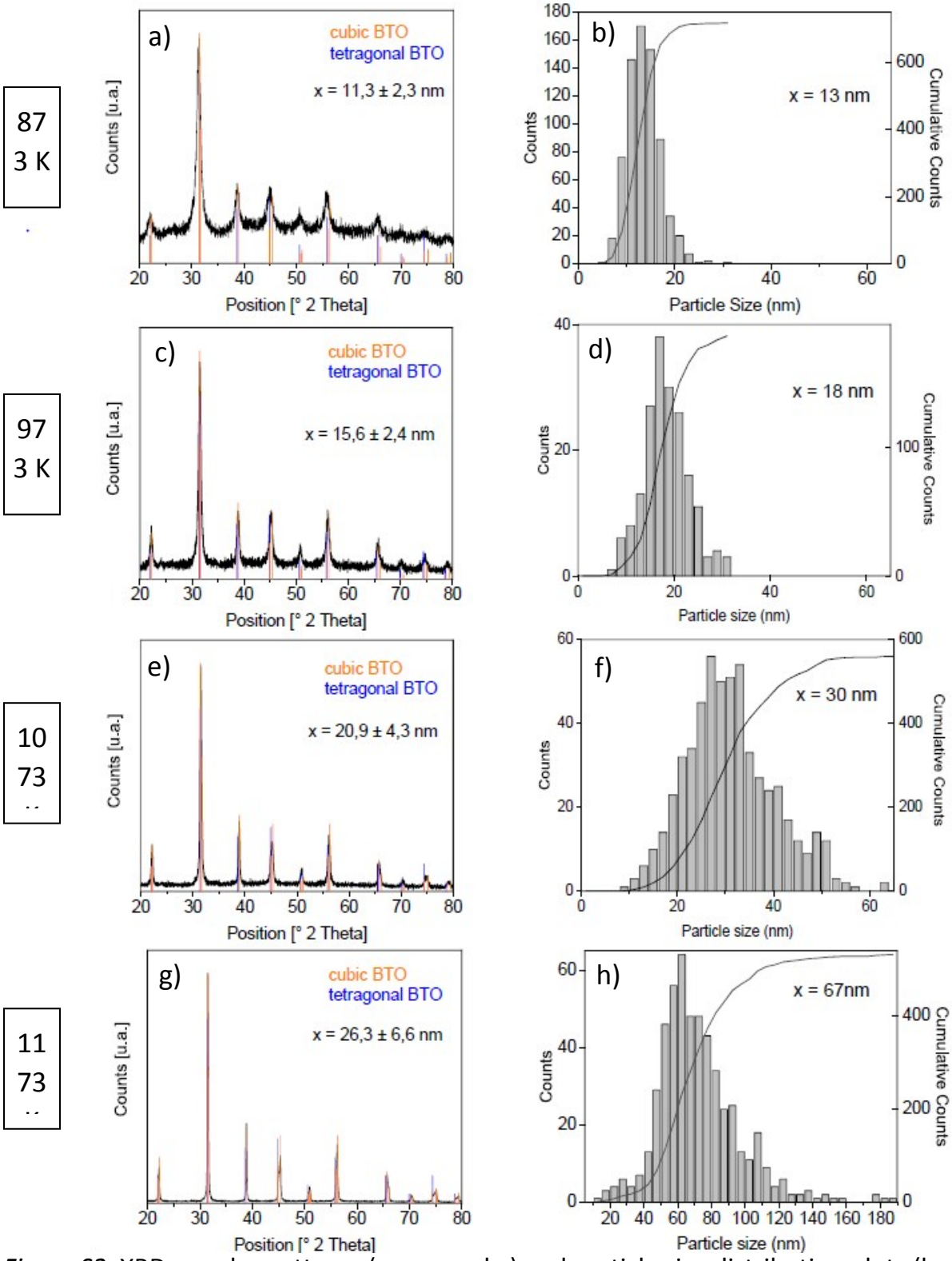


Figure S1. Temperature – pressure profiles for the BTO particle powder pre-annealing steps in the temperature range between T = 873 K (a) to T = 1173 K (d).

S2



87 3 K

97 3 K

10 73 ..

11 73 ..

Figure S2. XRD powder patterns (a, c, e and g) and particle size distribution plots (b, d, f and h) of $BaTiO_3$ nanoparticle powders pre-annealed at the temperatures between T = 873 K and 1173 K.

S3

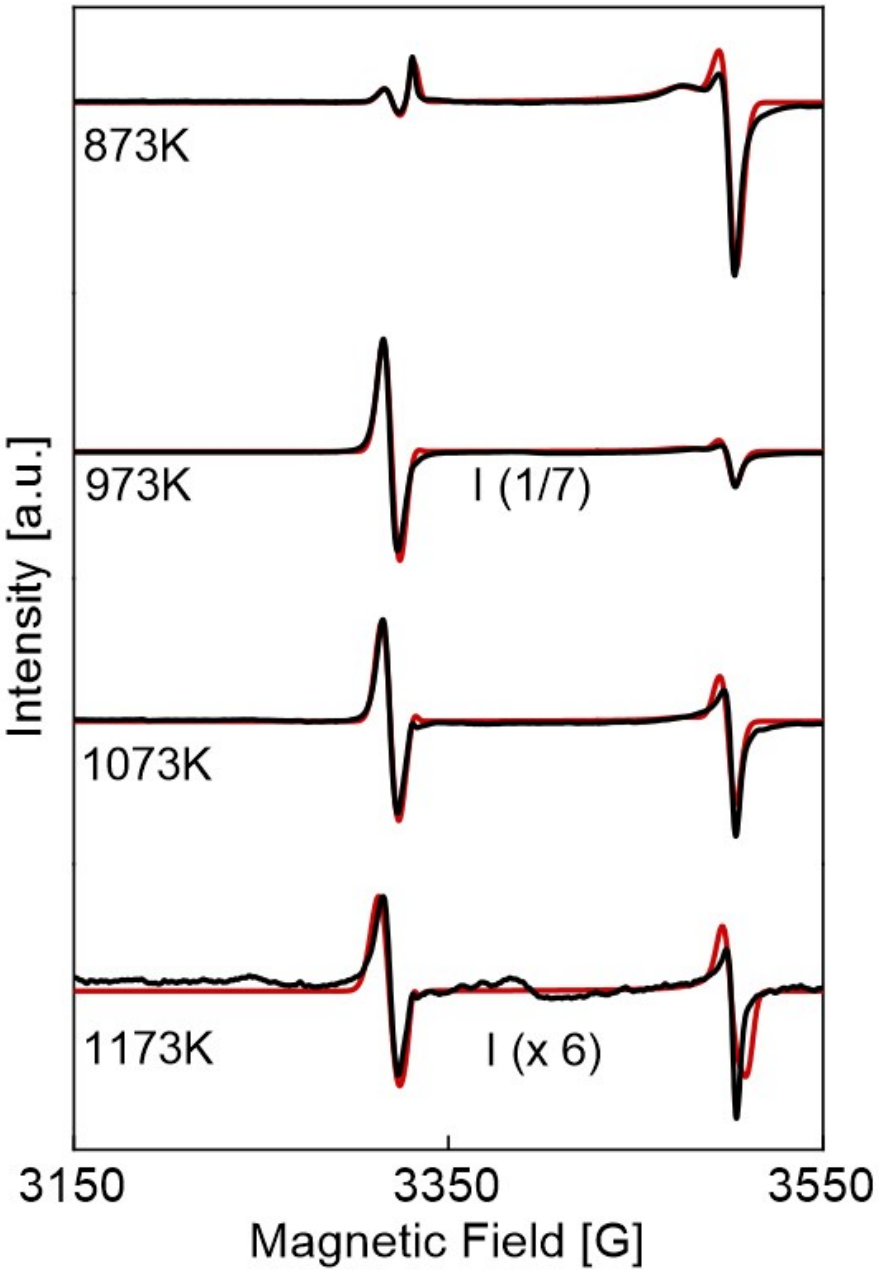


Figure S3. Experimental (black line) and simulated (red line) EPR spectra of $BaTiO_3$ nanoparticles after thermal pre-treatment in the temperature range of T = 873 K to 1173 K.

Table S1: Spin Hamiltonian of the EPR signals plotted in Figure 2(d-f) and Figure 3.

BTO 873K

	Spin System	g-values	g-strain	H-strain	lwpp (line width peak to peak)	weight
Ti^{3+} c-type axial symmetry	1/2	1.89973 1.9968		[22 10 0]	[0.47043]	17.0012
Ti^{3+} c-type othorombic symmetry	1/2	1.89951 1.91078 1.99745		[5 50 0]	[0.478379]	13.0003
Paramagnetic barium-oxygen divacancy	1/2	2.0039	[0.0063]		[0]	0.38
Ti^{3+} / electron center axial symmetry	1/2	1.9010 1.9060		[0 0 0.5]	[0.6]	0.30

BTO 973K

	Spin System	g-values	g-strain	H-strain	lwpp (line width peak to peak)	weight
Ti^{3+} c-type axial symmetry	1/2	1.89973 1.9968		[22 10 10]	[0.47043]	17.0012
Ti^{3+} c-type othorombic symmetry	1/2	1.899 1.9097 1.9968		[5 50 0]	[0.5]	20
Paramagnetic barium-oxygen divacancy	1/2	2.0039	[0.0063]		[0]	21
Ti^{3+} / electron center axial symmetry	1/2	1.9005 1.9040		[0 0 0.5]	[0.6]	0.8

BTO 1073K

	Spin System	g-values	g-strain	H-strain	lwpp (line width peak to peak)	weight
Ti^{3+} c-type axial symmetry	1/2	1.89973 1.9968		[22 10 0]	[0.4]	5
Ti^{3+} c-type othorombic symmetry	1/2	1.8985 1.9099 1.9968		[5 50 0]	[0.4]	3
Paramgnetic barium-oxygen divacancy	1/2	2.0042	[0.0064]		[0]	3
Ti3+ / electron center axial symmetry	1/2	1.8999 1.9040		[0 0 0.5]	[0.6]	0.8

BTO 1173K

	Spin System	g-values	g-strain	H-strain	lwpp (line width peak to peak)	weight
Ti^{3+} c-type axial symmetry	1/2	1.9032 2.0014		[22 10 0]	[0.32]	1.8
Ti^{3+} c-type othorombic symmetry						
Paramgnetic barium-oxygen divacancy	1/2	2.009	[0.008]		[0]	0.63
Ti3+ / electron center axial symmetry	1/2	1.8999 1.9070		[0 0 0.5]	[0.6]	0.20