

Electronic Supplementary Information (ESI):

On the formation of superoxide radicals on colloidal ATiO_3 (A = Sr and Ba) nanocrystal surfaces

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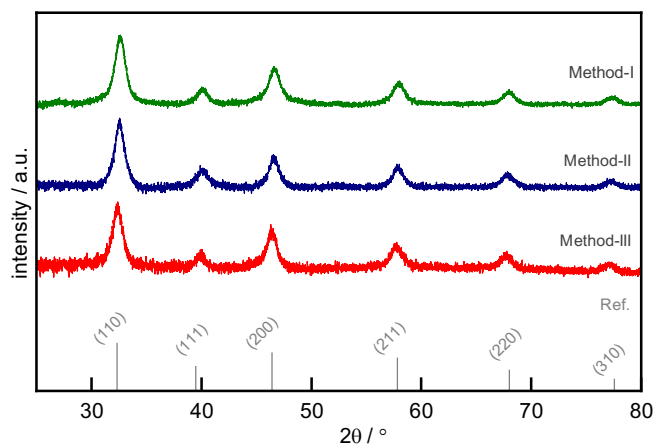


Fig. S1. Powder X-ray diffraction patterns of SrTiO_3 NCs prepared from all three methods indexed to the cubic phase of bulk SrTiO_3 with $\text{Pm}\bar{3}\text{m}$ space group.¹

Table S1. The average lattice parameter and crystallite size calculated using Rigaku SmartLab Studio II for all three samples.

Preparation Method	Lattice parameter (Å)	Crystallite size (nm) [†]
I (aerobic without hydrazine)	3.9069	7.3 ± 0.3
II (aerobic with hydrazine)	3.9162	7.5 ± 0.4
III (anaerobic without hydrazine)	3.9163	7.6 ± 0.7

[†]Crystallite size is the average size calculated from the three most intense reflections: (110), (200) and (211).

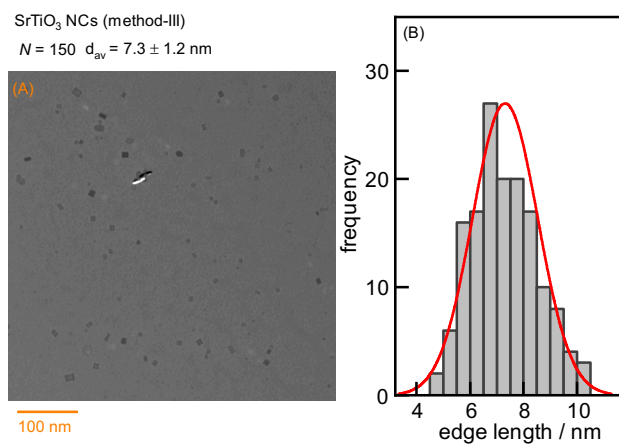


Fig. S2. Representative transmission electron microscopy (TEM) image of SrTiO₃ NCs prepared from method III (degassed with argon) showing a clear cubic morphology of NCs. The size distribution plot from analyzing over hundred different particles in raw TEM image using ImageJ software displays an average size of 7.3 ± 1.2 nm in good agreement with crystallite size calculated from diffraction pattern in Figure S1. The cubic morphology of NCs prepared from the method I and method II is already confirmed in our previous report.²

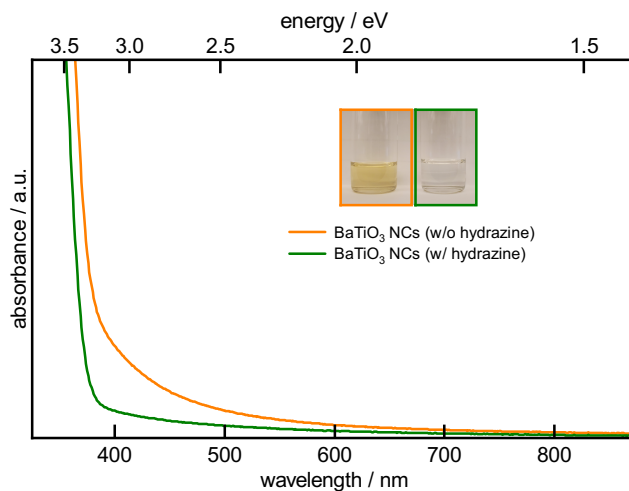


Fig. S3. Room temperature electronic absorption spectra of BaTiO₃ NCs prepared from method-A (without hydrazine/orange) and method-B (with hydrazine/green). The color photographs of both samples are shown in inset.

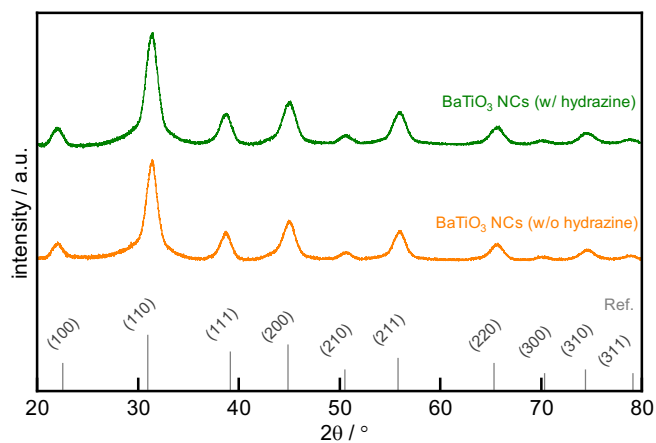


Fig. S4. Powder X-ray diffraction pattern of BaTiO₃ NCs prepared from method-A (without hydrazine/orange) and method-B (with hydrazine/green) indexed to cubic phase of BaTiO₃.³

Table S2. The average lattice parameter and crystallite size calculated using Rigaku SmartLab Studio II for both samples.

Sample NCs	Lattice parameter (Å)	Crystallite size (nm) [†]
With hydrazine	4.0230	5.66 ± 0.50
Without hydrazine	4.0335	6.54 ± 0.53

[†]Crystallite size is the average size calculated from the three most intense reflections: (110), (200) and (211).

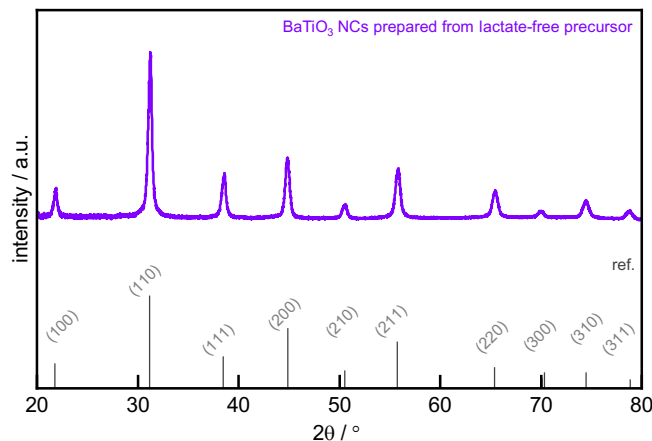


Fig. S5. Powder X-ray diffraction pattern of BaTiO₃ NCs prepared from lactate-free method indexed to cubic phase of single crystal BaTiO₃.

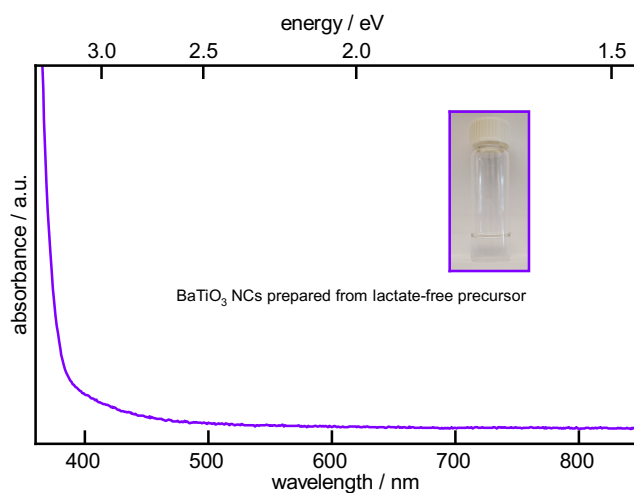


Fig. S6. Room temperature electronic absorption spectrum of BaTiO₃ NCs prepared from lactate-free precursor. The color photograph of hexanes solution of as-prepared NCs is shown in inset.

References:

1. R. Mitchell, A. Chakhmouradian and P. Woodward, Crystal chemistry of perovskite-type compounds in the tausonite-loparite series, $(\text{Sr}_{1-2x}\text{Na}_x\text{La}_x)\text{TiO}_3$, *Phys. Chem. Miner.*, 2000, 27(8), 583.
2. W. L. Harrigan, S. E. Michaud, K. A. Lehuta and K. R. Kittilstved, Tunable electronic structure and surface defects in chromium-doped colloidal SrTiO_{3-δ} nanocrystals, *Chem. Mater.*, 2016, 28(2), 430.
3. M. B. Smith, K. Page, T. Siegrist, P. L. Redmond, E. C. Walter, R. Seshadri, L. E. Brus and M. L. Steigerwald, Crystal structure and the paraelectric-to-ferroelectric phase transition of nanoscale BaTiO₃, *J. Am. Chem. Soc.*, 2008, 130(22), 6955.