

Supplementary Information for “Stabilization Mechanism of the Tetragonal Structure in a Hydrothermally Synthesized BaTiO₃ Nanocrystal”

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Modelling

This supporting information gives all the possible patterns of *cis*- and *trans*-configurations in $\text{Ba}_{1-0.5x}\text{TiO}_{3-x}\text{OH}_x$ supercells with stoichiometric substitutions of $x = 0.07/0.17/0.50/0.67$, while only the most stable configurations for each of the substitutions are given in the maintext. Figures S-1, S-2, S-3, and S-4 correspond to the supercells of $x = 0.07, 0.17, 0.50$ and 0.67 , respectively.

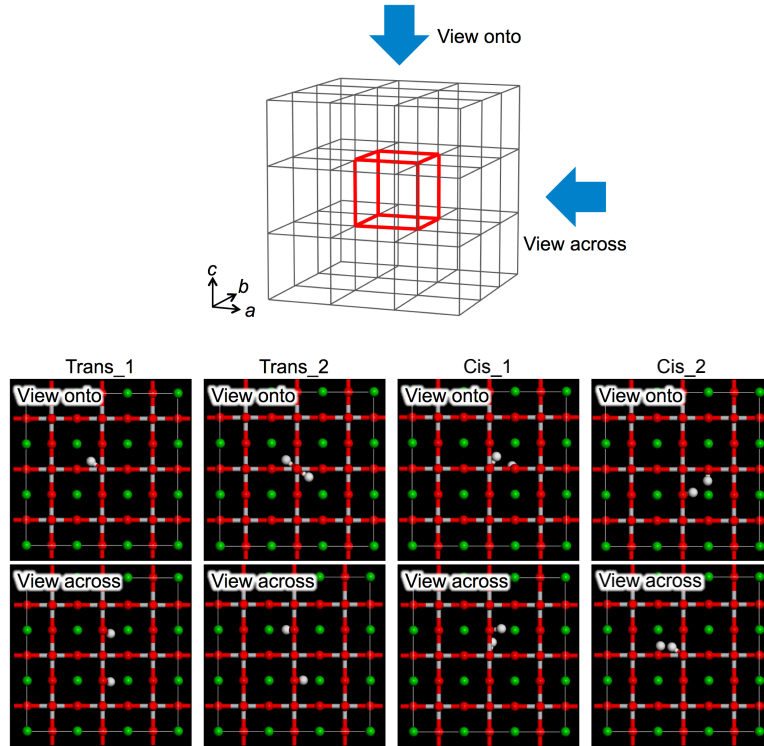


Figure S-1: All the possible patterns of *cis*- and *trans*-configurations in $3 \times 3 \times 3$ $\text{Ba}_{1-0.5x}\text{TiO}_{3-x}\text{OH}_x$ supercell with $x = 0.07$ substitution. The *trans*-models of *a*- and *c*-axis orientations were generated by changing the axial direction of the supercell without changing the atomic arrangement.

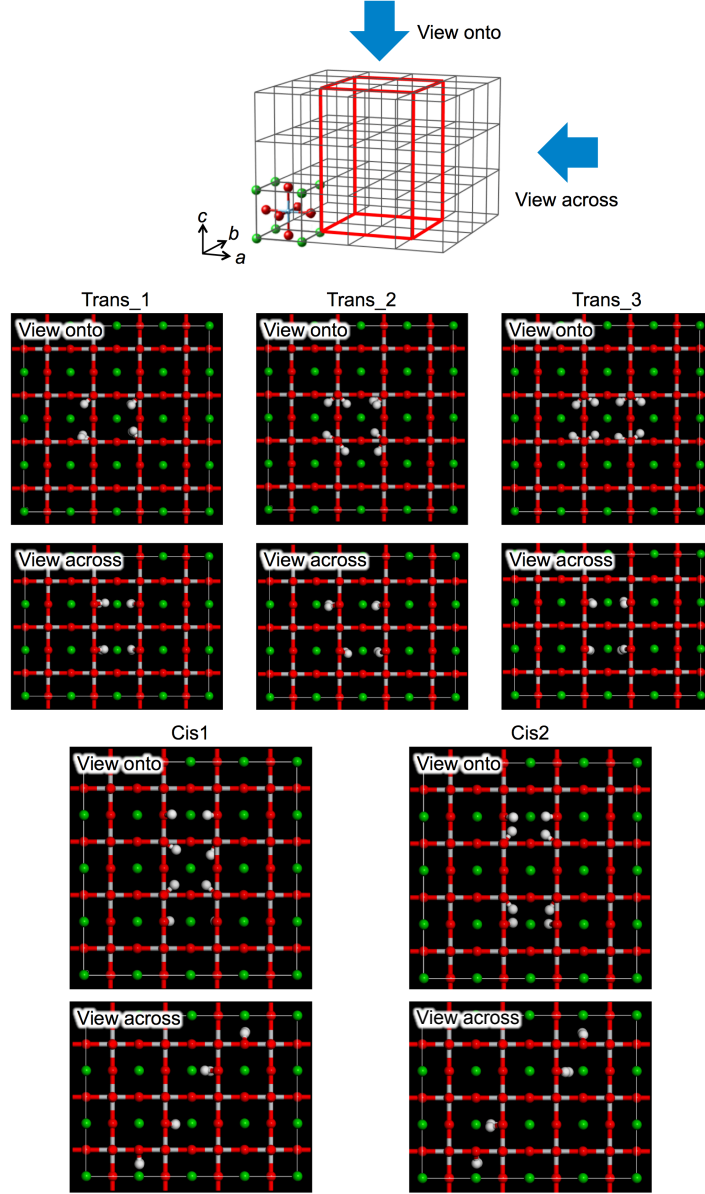


Figure S-2: All the possible patterns of *cis*- and *trans*-configurations in $4 \times 4 \times 3$ $\text{Ba}_{1-0.5x}\text{TiO}_{3-x}\text{OH}_x$ supercell with $x = 0.17$ substitution. The *trans*-models of *a*- and *c*-axis orientations were generated by changing the axial direction of the supercell without changing the atomic arrangement.

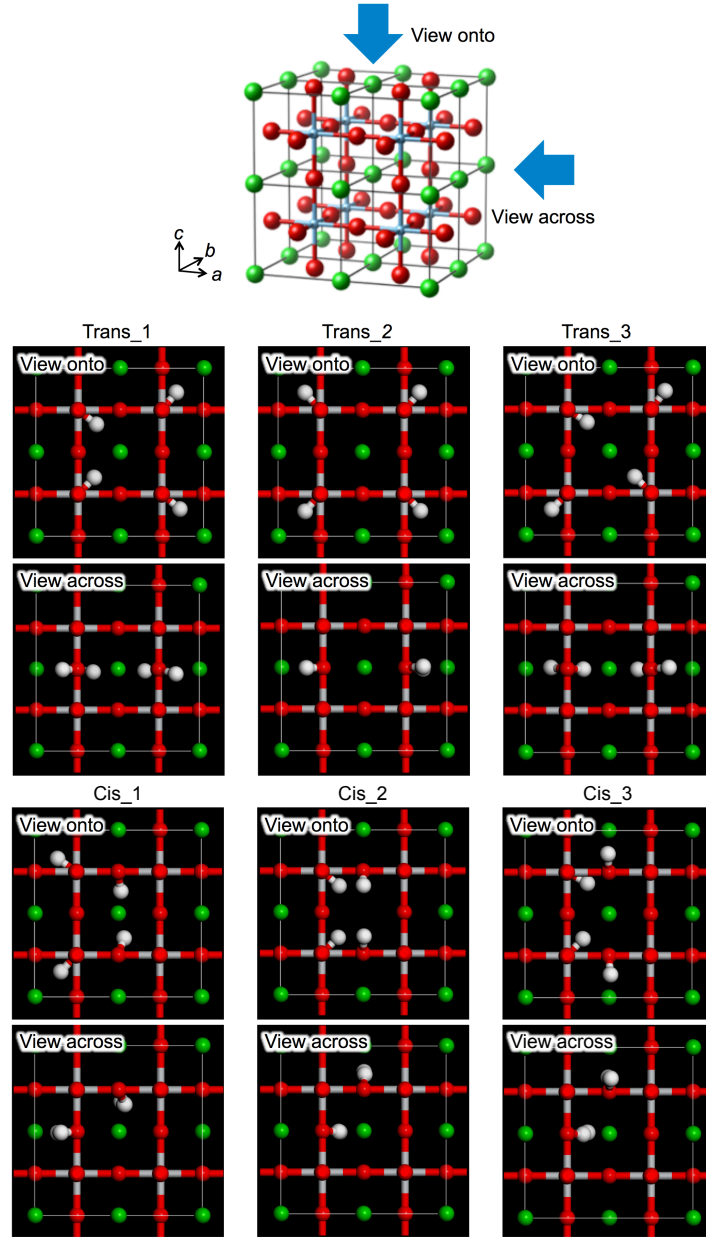


Figure S-3: All the possible patterns of *cis*- and *trans*-configurations in $2 \times 2 \times 2$ $\text{Ba}_{1-0.5x}\text{TiO}_{3-x}\text{OH}_x$ supercell with $x = 0.50$ substitution. The *trans*-models of *a*- and *c*-axis orientations were generated by changing the axial direction of the supercell without changing the atomic arrangement.

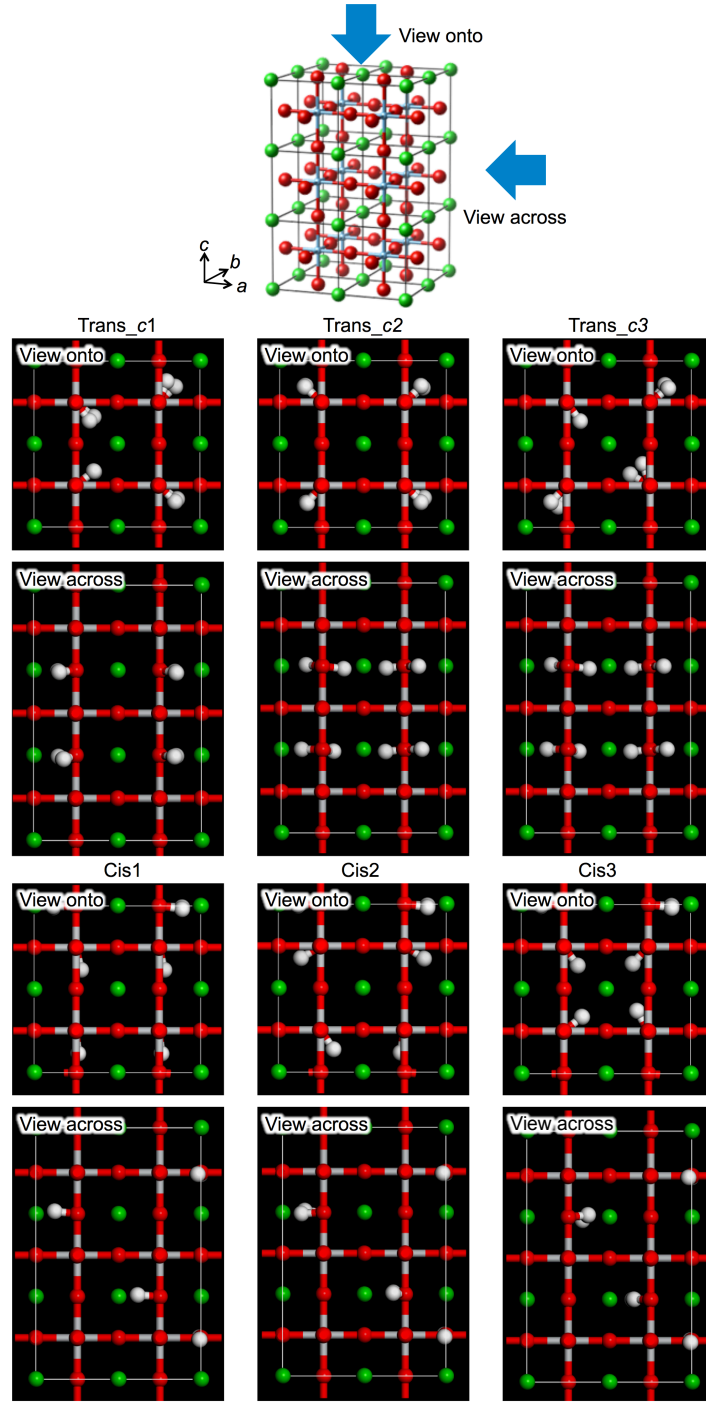


Figure S-4: All the possible patterns of *cis*- and *trans*-configurations in $2 \times 2 \times 3$ $\text{Ba}_{1-0.5x}\text{TiO}_{3-x}\text{OH}_x$ supercell with $x = 0.67$ substitution. The *trans*-models of *a*- and *c*-axis orientations were generated by changing the axial direction of the supercell without changing the atomic arrangement.