A-site Cation Bulk and Surface Diffusion in A-site-deficient $BaZrO_3$ and $SrZrO_3$ Perovskites

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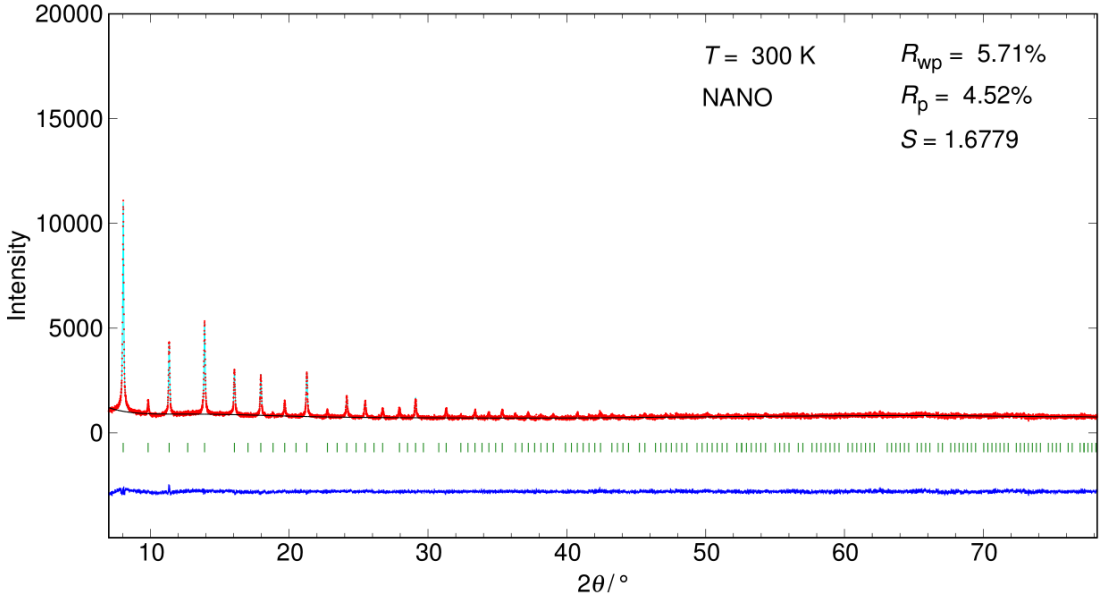
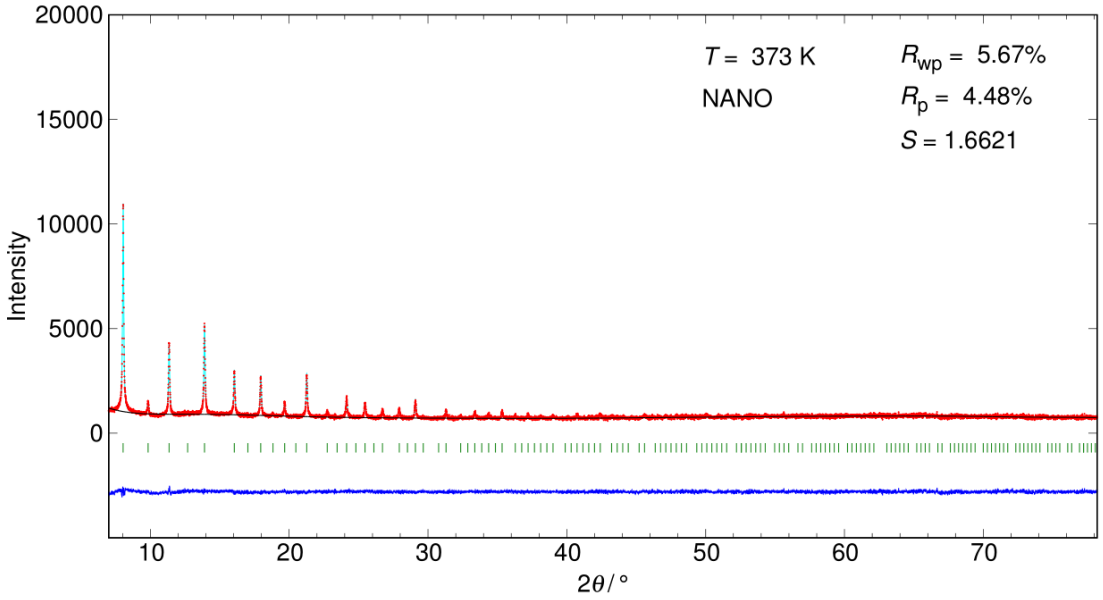
Supplementary Information

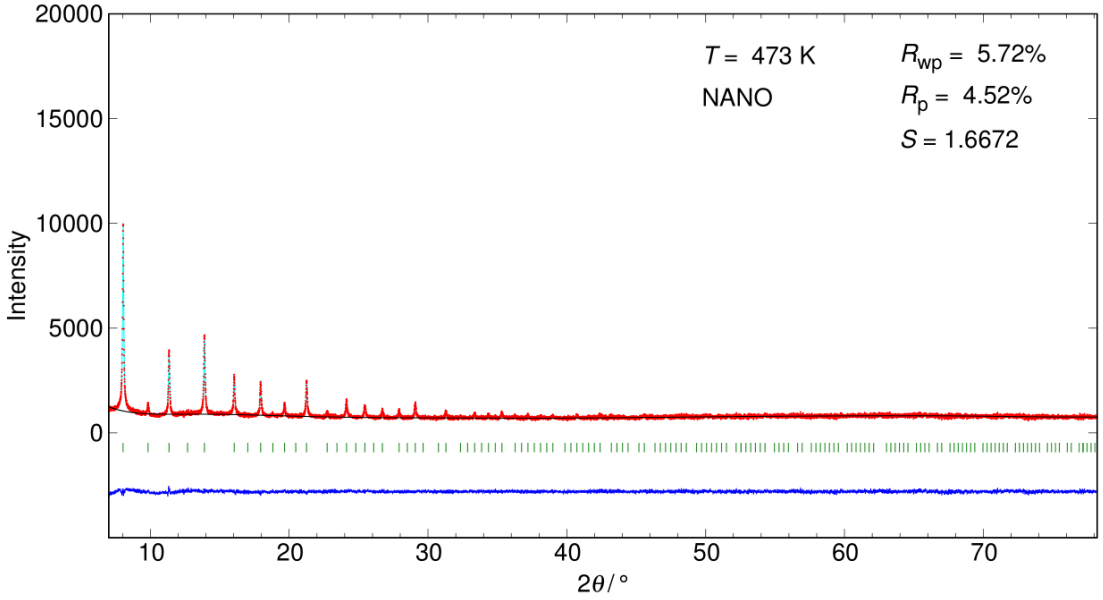
(A)



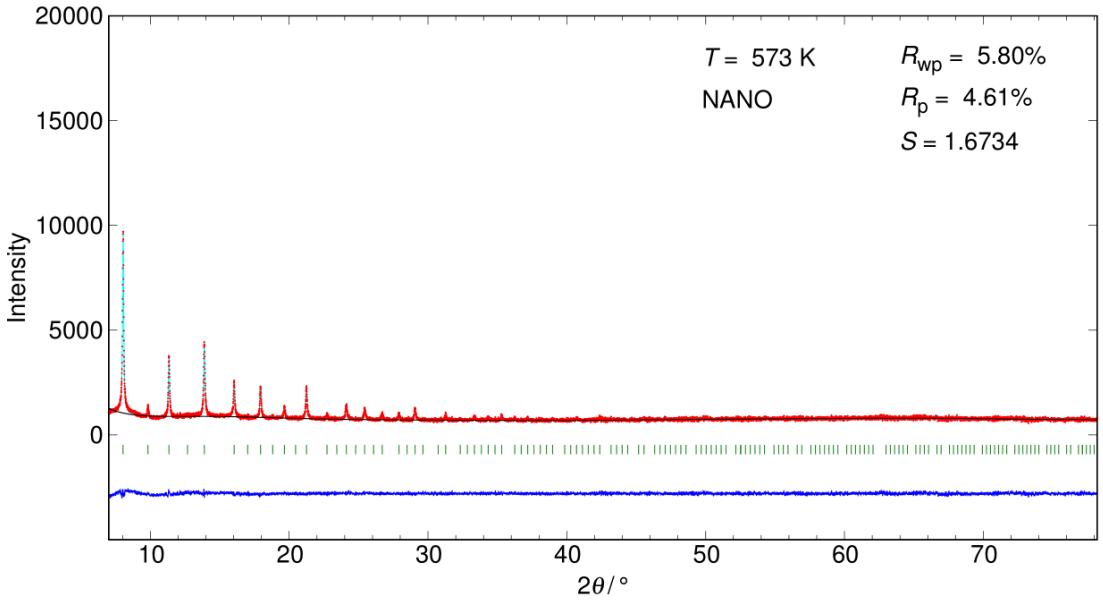
(B)


T = 373 K
NANO
R_{wp} = 5.67%
R_p = 4.48%
S = 1.6621
Intensity
2θ/°

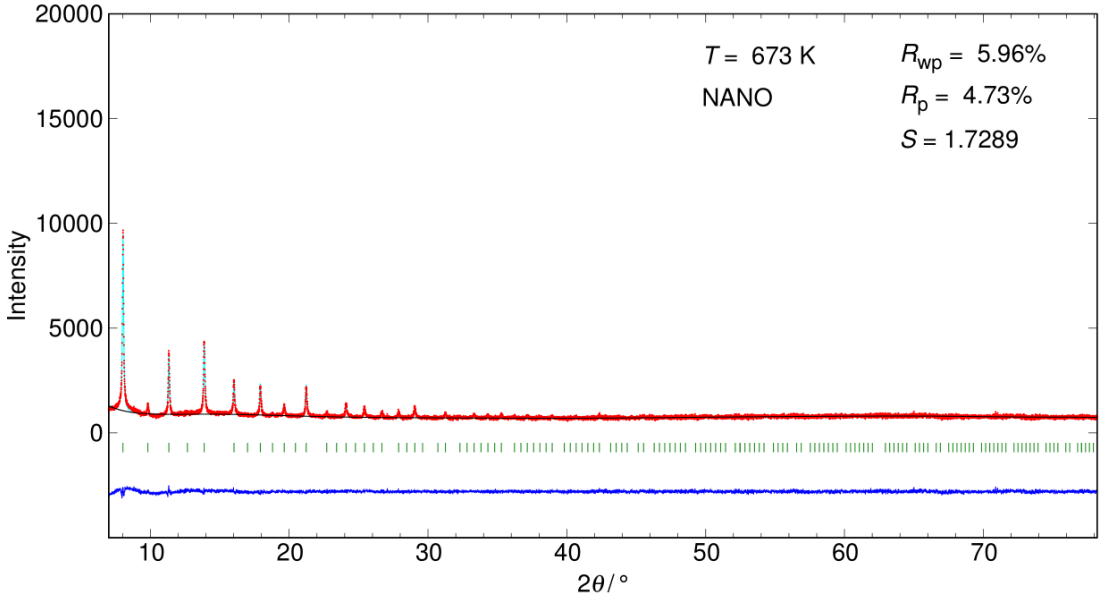
(C)


T = 473 K
NANO
R_{wp} = 5.72%
R_p = 4.52%
S = 1.6672
Intensity
2θ/°

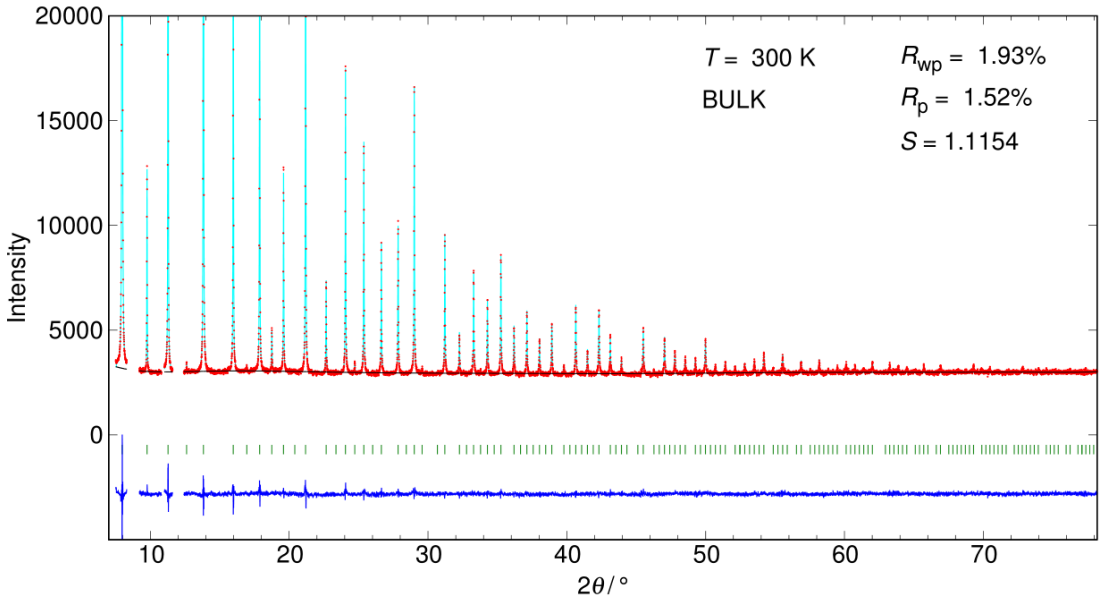
(D)


T = 573 K
NANO
R_{wp} = 5.80%
R_p = 4.61%
S = 1.6734
Intensity
2θ/°

(E)


T = 673 K
NANO
R_{wp} = 5.96%
R_p = 4.73%
S = 1.7289
Intensity
2θ/°

(F)



(G)

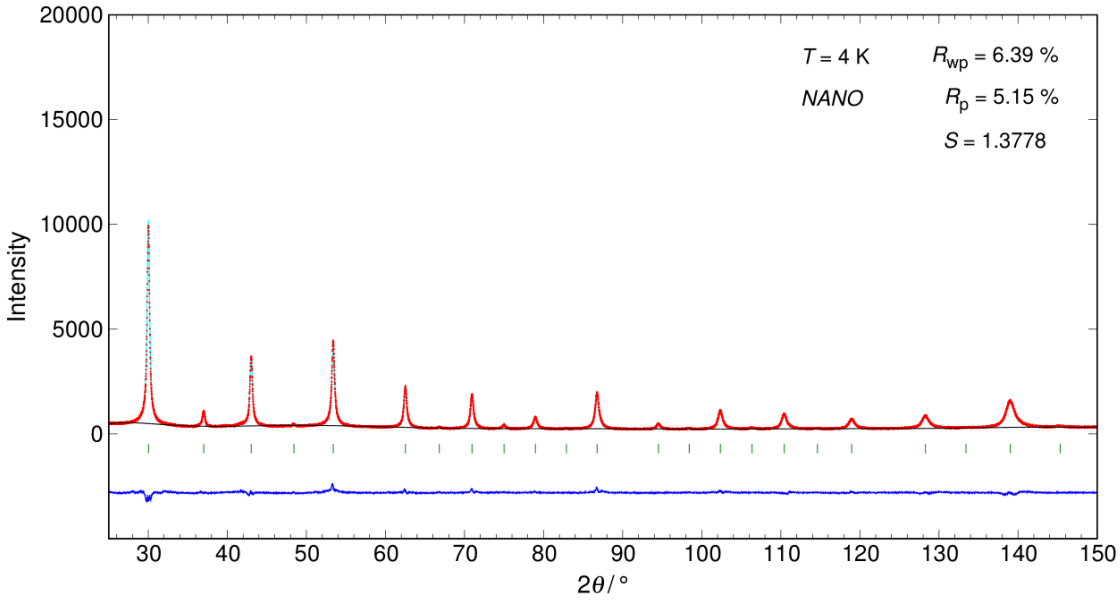


Figure S1 Synchrotron X-ray diffraction and Rietveld fitting results for $BaZrO_3$ nanoparticles at (A) 300 K, (B) 373 K, (C) 473 K, (D) 573 K, and (E) 673 K, and (F) bulk $BaZrO_3$ at 300 K. (G) CuKα1 characteristic X-ray for low temperature (4 K) diffraction for nano. The red plots represent experimental diffraction patterns, the light blue lines show the fitting patterns, and the black line is the refined background. The vertical bars show the peak positions of $BaZrO_3$ (space group 221, Pm-3m) and the blue curve beneath it shows the fitting residues.

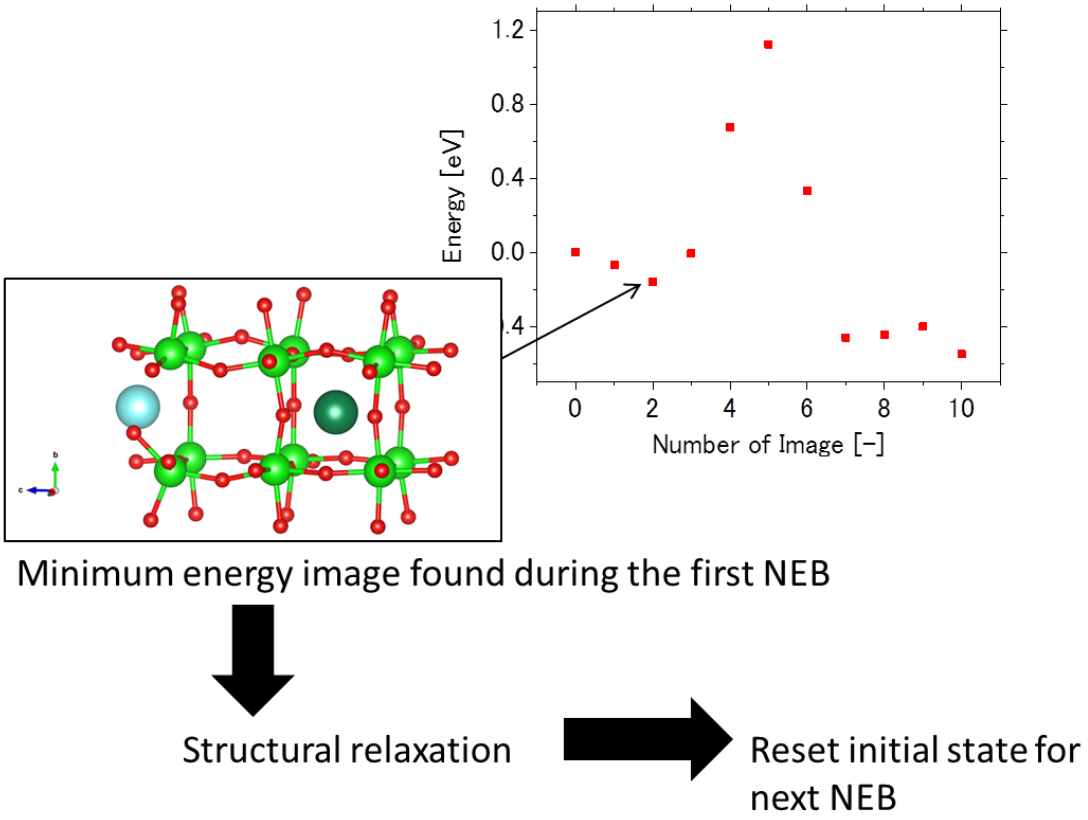


Figure S2 Iteration process of NEB calculations when more stable configurations than the initial one are found.