Supporting Information for

Solution-Phase Synthesis of Alloyed $Ba(Zr_{1-x}Ti_x)S_3$ Perovskite and Non-Perovskite Nanomaterials

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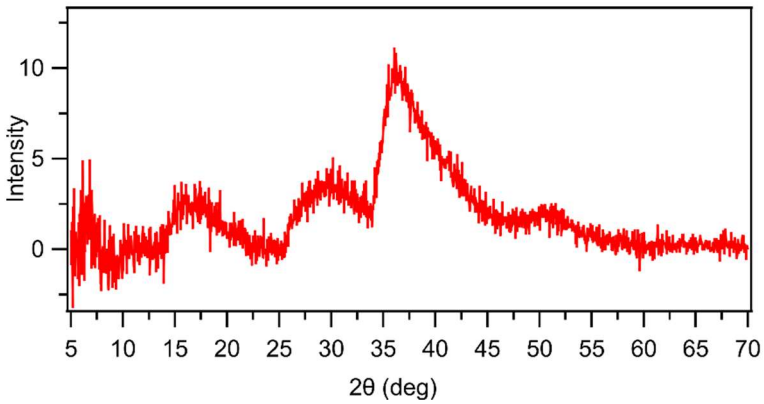

Figure S1. Representative powder X-ray diffraction (XRD) blank measured on a "zero-background" silicon plate, showing some background scattering from the instrument and sample holder. The data presented in the text, unless otherwise stated, was processed by subtracting a background scan acquired under the same conditions and applying a simple polynomial background correction.

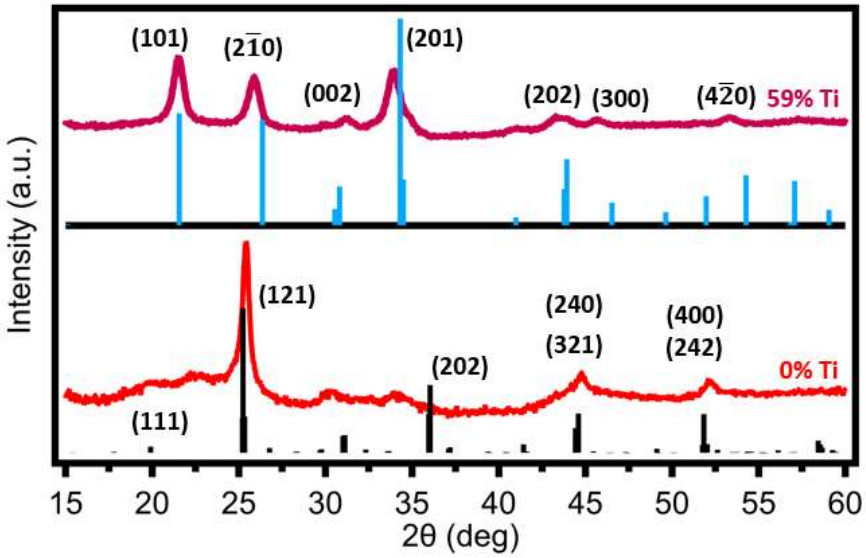

Figure S2. Powder X-ray diffraction (XRD) pattern for samples with low and high titanium alloying showing the Miller indices corresponding to selected prominent peaks in the accompanying reference patterns. These patterns are accompanied by the calculated reference patterns for $BaZrS_3$ in the *Pnma* crystal structure and $BaTiS_3$ in the *P6₃/mmc* crystal structure.

LeBail Refinement of PXRD Data. LeBail refinement of the PXRD data of alloyed nanoparticles was used as an approach to systematically extract the lattice constants for the orthorhombic (*Pnma*) or hexagonal (*P6₃/mmc*) phase nanocrystals. GSAS-II was used for fitting. The background (shown as the red curve in the figures below) was fitted as the combination of three contributions: a fixed contribution from a measured background scan for a blank sample plate; a 3rd-order polynomial (Chebyschev-1 background function) and a background peak corresponding to contributions from scattering from amorphous components of the sample (such as excess ligands), which is generally a broad peak centered at approximately 20.6°. Other parameters that were allowed to refine were: the lattice constants (a, b, and c for the orthorhombic phase or a and c for the hexagonal phase); a sample displacement parameter; and peakwidth as a result of domain size, according to a uniaxial domain size model. The unique axis was taken to be [010] for the orthorhombic crystals and [001] for the hexagonal crystals, in accordance with our prior results and the best fit to the data.

Table S1. LeBail Refinement Parameters[a]

ICP Ti%	Fit Phase	*a* (Å)	*b* (Å)	*c* (Å)	Cell Volume (Å^3)	Sample Disp. (μm)	Equatorial Size (nm)	Axial Size (nm)	R
0	*Pnma*	6.997(7)	10.25(1)	7.012(3)	503.0(8)	-10(20)	24.5(8)	2.8(1)	2.2%
9	*Pnma*	6.977(4)	10.16(2)	7.009(6)	497(1)	13(30)	18(1)	2.0(1)	1.8%
11	*Pnma*	6.970(2)	10.132(6)	7.009(2)	495.0(4)	-90(13)	47(1)	4.5(1)	1.9%
11[b]	*P6₃/mmc*	6.999(3)	--	4.99(1)	211.6(6)	-152(7)	20.3(3)	1.8(1)	2.5%
15	*P6₃/mmc*	6.957(3)	--	5.806(5)	243.4(2)	105(8)	21.1(4)	3.0(1)	1.8%
18	*P6₃/mmc*	6.951(3)	--	5.806(6)	242.9(3)	7(7)	24.1(5)	3.2(1)	2.4%
24	*P6₃/mmc*	6.915(2)	--	5.874(3)	243.5(1)	117(5)	31.4(5)	8.8(2)	2.2%
35	*P6₃/mmc*	6.877(3)	--	5.880(2)	241.0(1)	22(7)	27.4(5)	9.6(2)	2.4%
59	*P6₃/mmc*	6.878(2)	--	5.729(1)	234.7(1)	28(7)	11.2(1)	9.6(1)	2.3%

[a]Numbers shown in parentheses are the esd's on the last digit of the given value. [b]This sample was assigned to the orthorhombic *Pnma* phase (see main text) but a fit to the hexagonal phase was also attempted for comparison. This gave a somewhat higher R-value than the orthorhombic phase, and, notably, an implausibly small value of *c*, suggesting that assignment to the orthorhombic phase is more plausible.

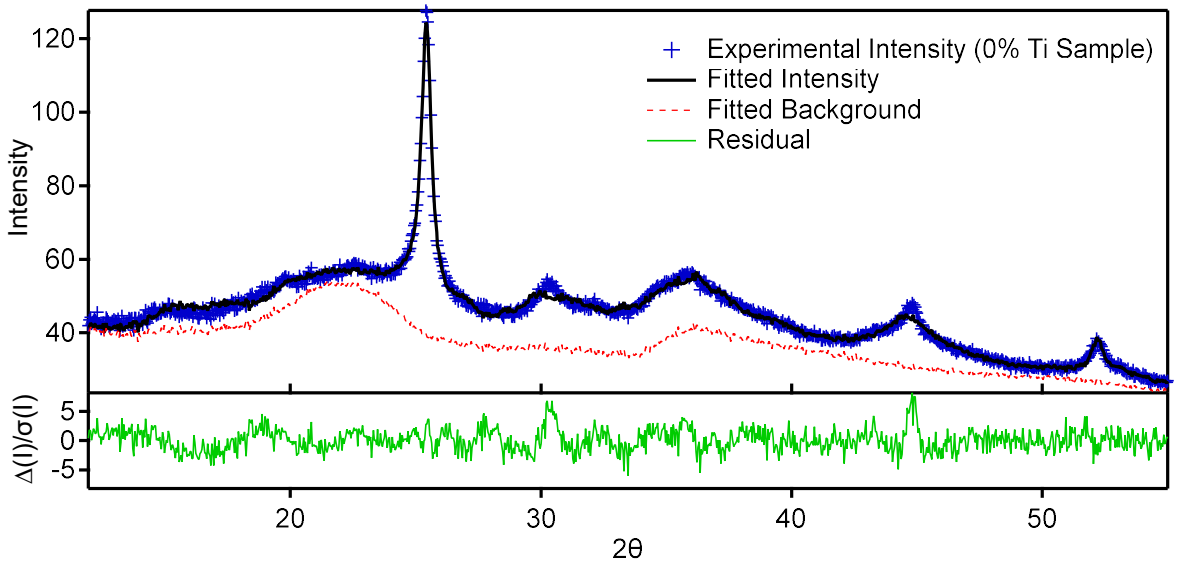

Figure S3. PXRD data and LeBail fit for unalloyed $BaZrS_3$ sample.

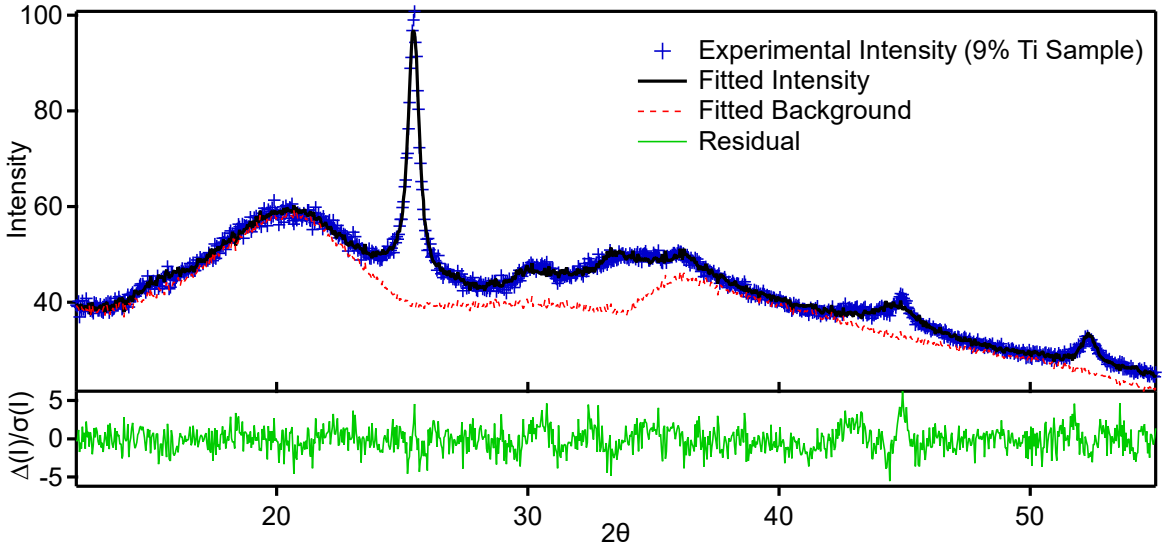

Figure S4. PXRD data and LeBail fit 9% Ti sample.

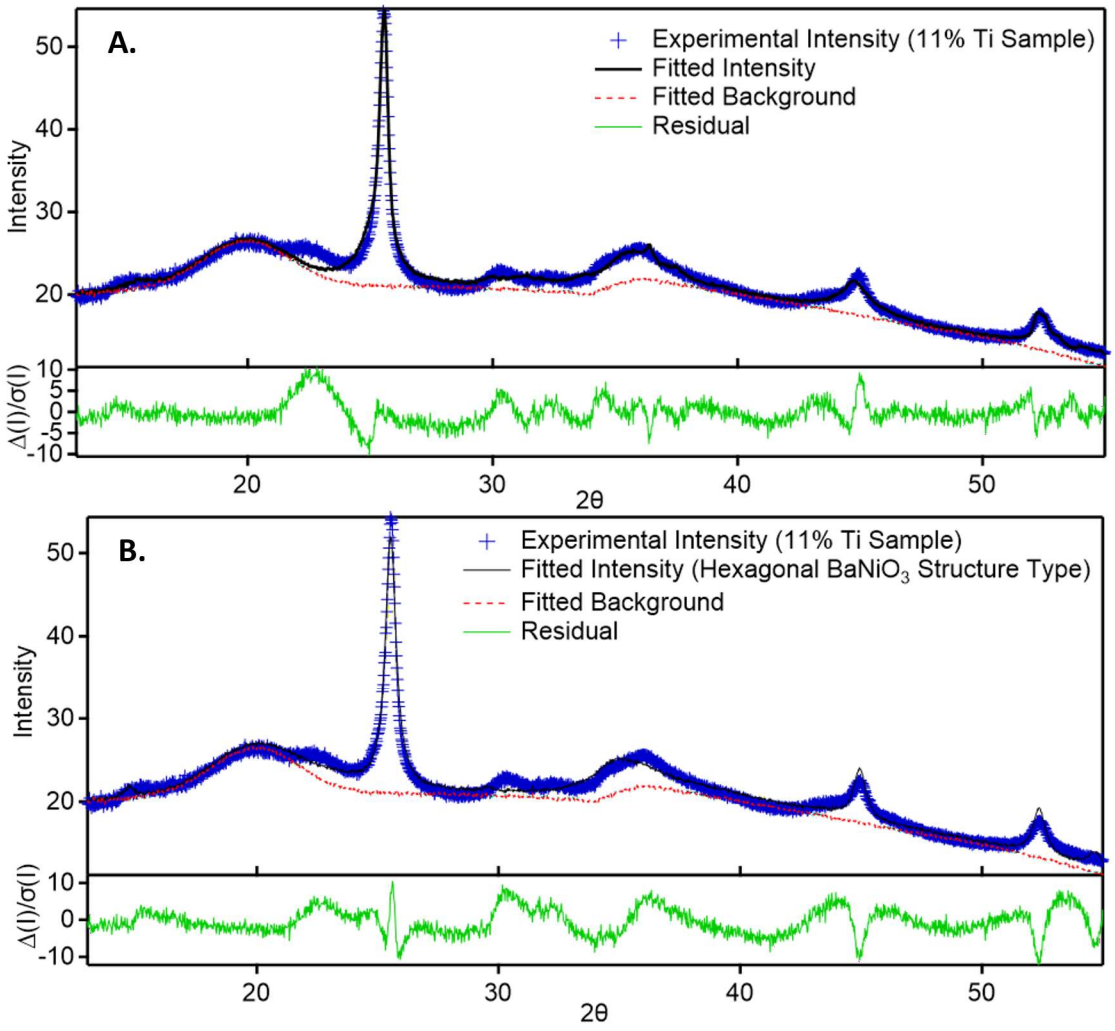

Figure S5. PXRD data and LeBail fit for 11% Ti sample, fit to the orthorhombic perovskite (*Pnma*) phase (**A**) or hexagonal phase (**B**).

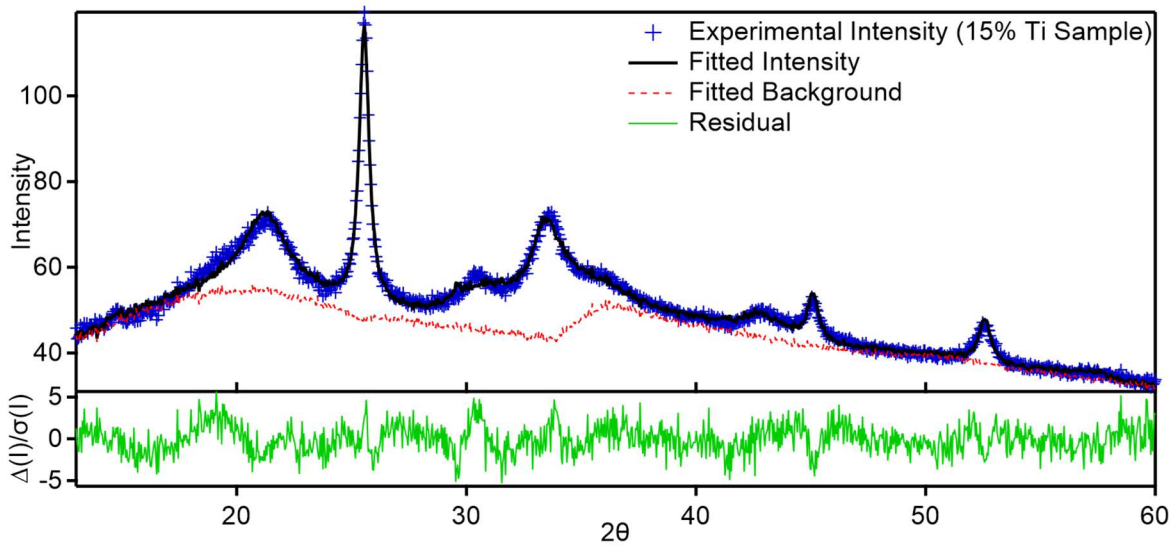

Figure S6. PXRD data and LeBail fit for 15% Ti sample.

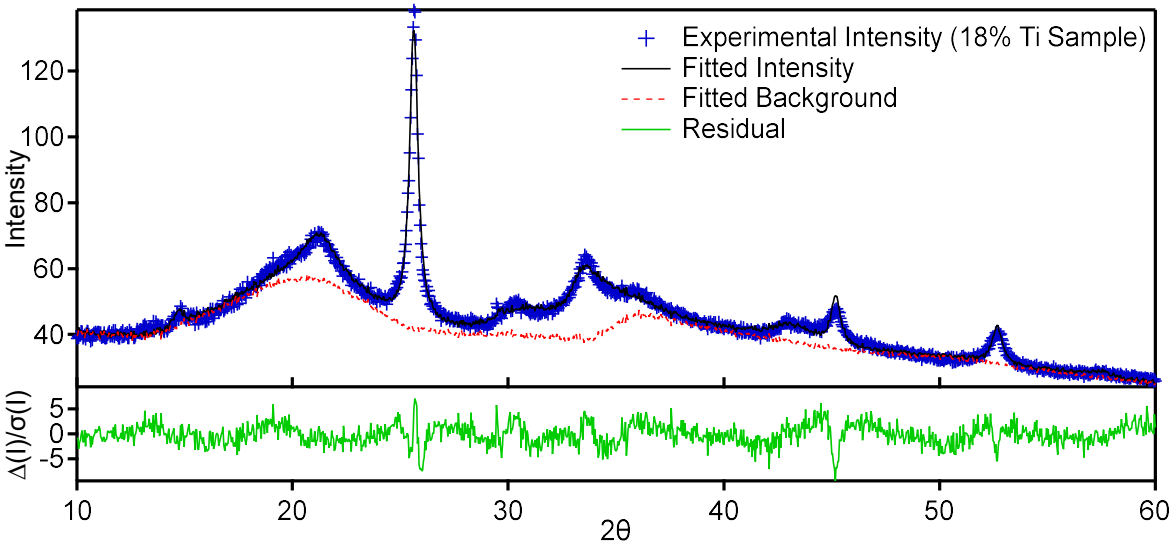

Figure S7. PXRD data and LeBail fit for 18% Ti sample.

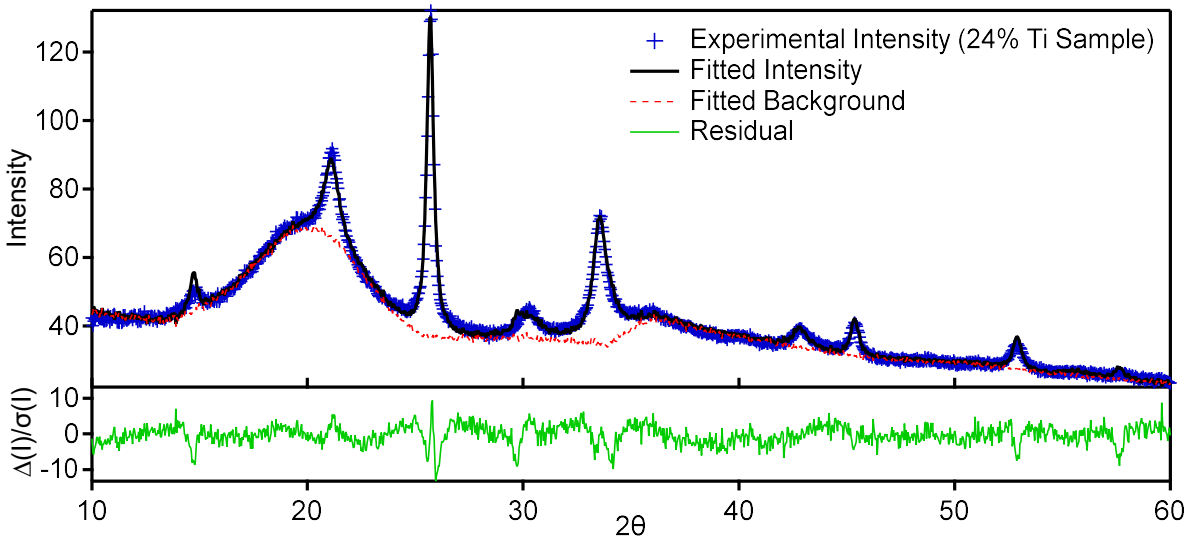

Figure S8. PXRD data and LeBail fit for 24% Ti sample.

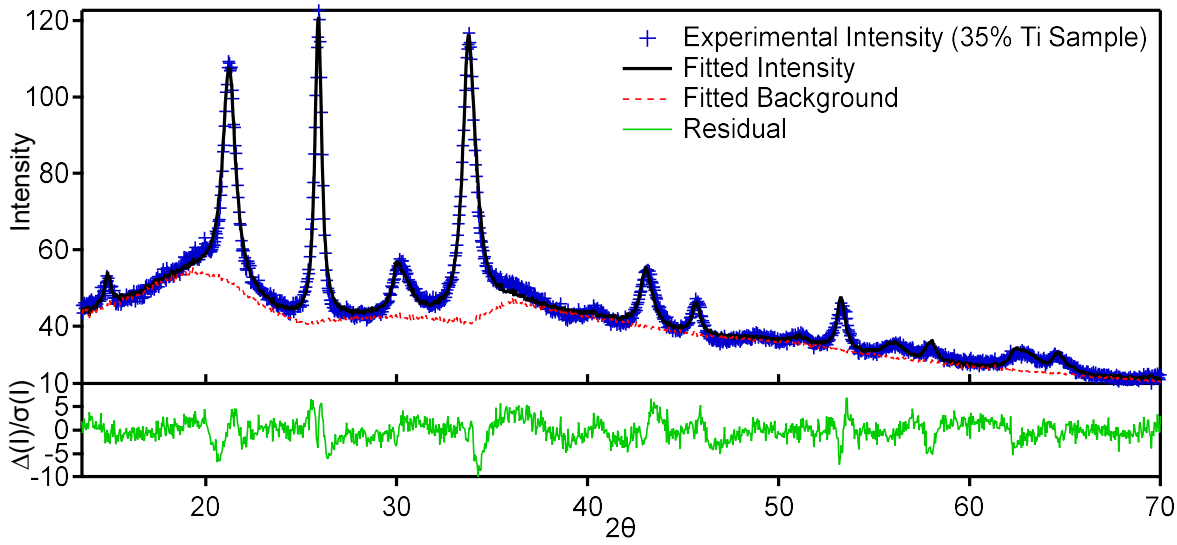

Figure S9. PXRD data and LeBail fit for 35% Ti sample.

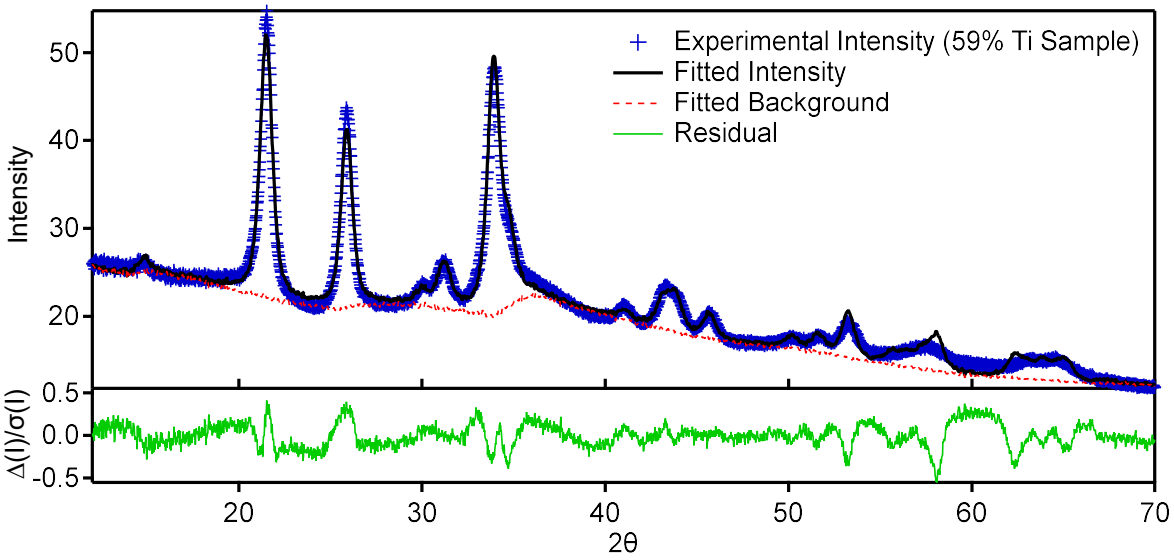

Figure S10. PXRD data and LeBail fit for 59% Ti sample.

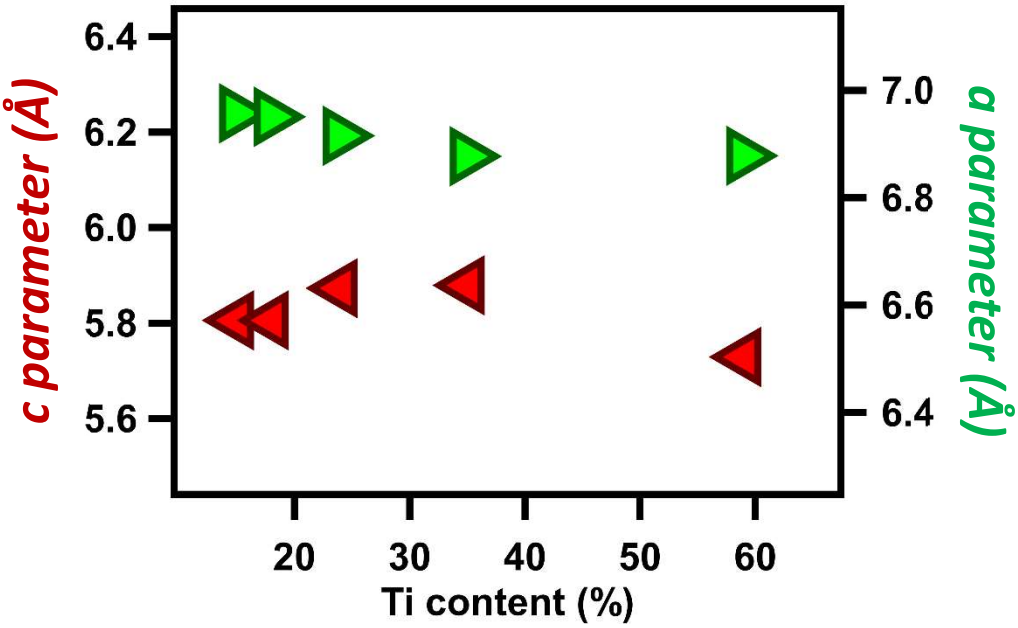

Figure S11. Fitted values of the *a* and *c* lattice parameters for nanocrystals in the hexagonal phase.

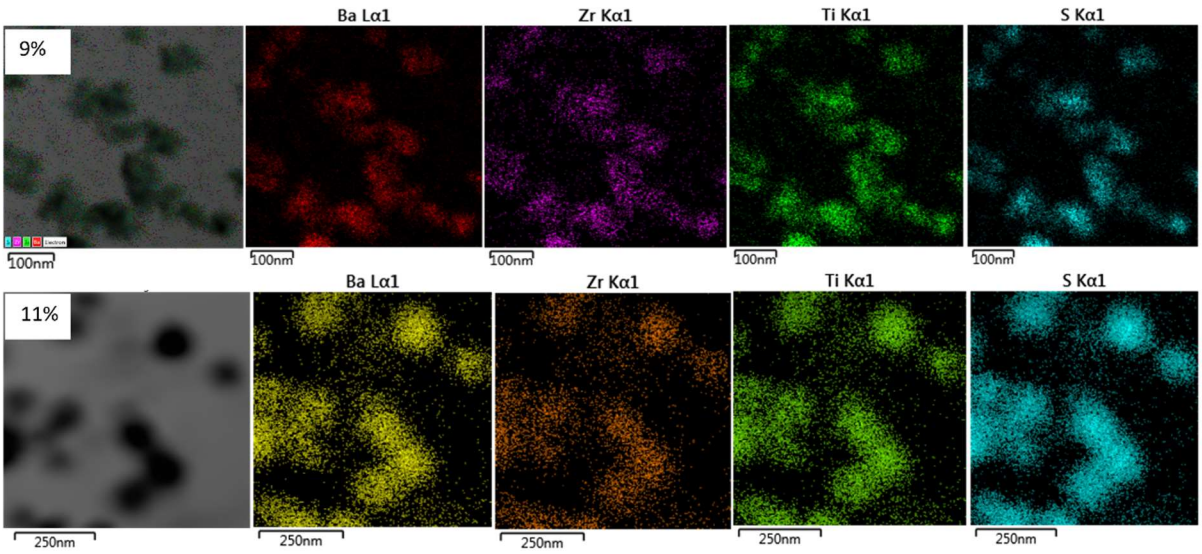

Figure S12. EDX mapping for $Ba(Zr_{1-x}Ti_x)S_3$ nanocrystal samples with 9% and 11% Ti content.

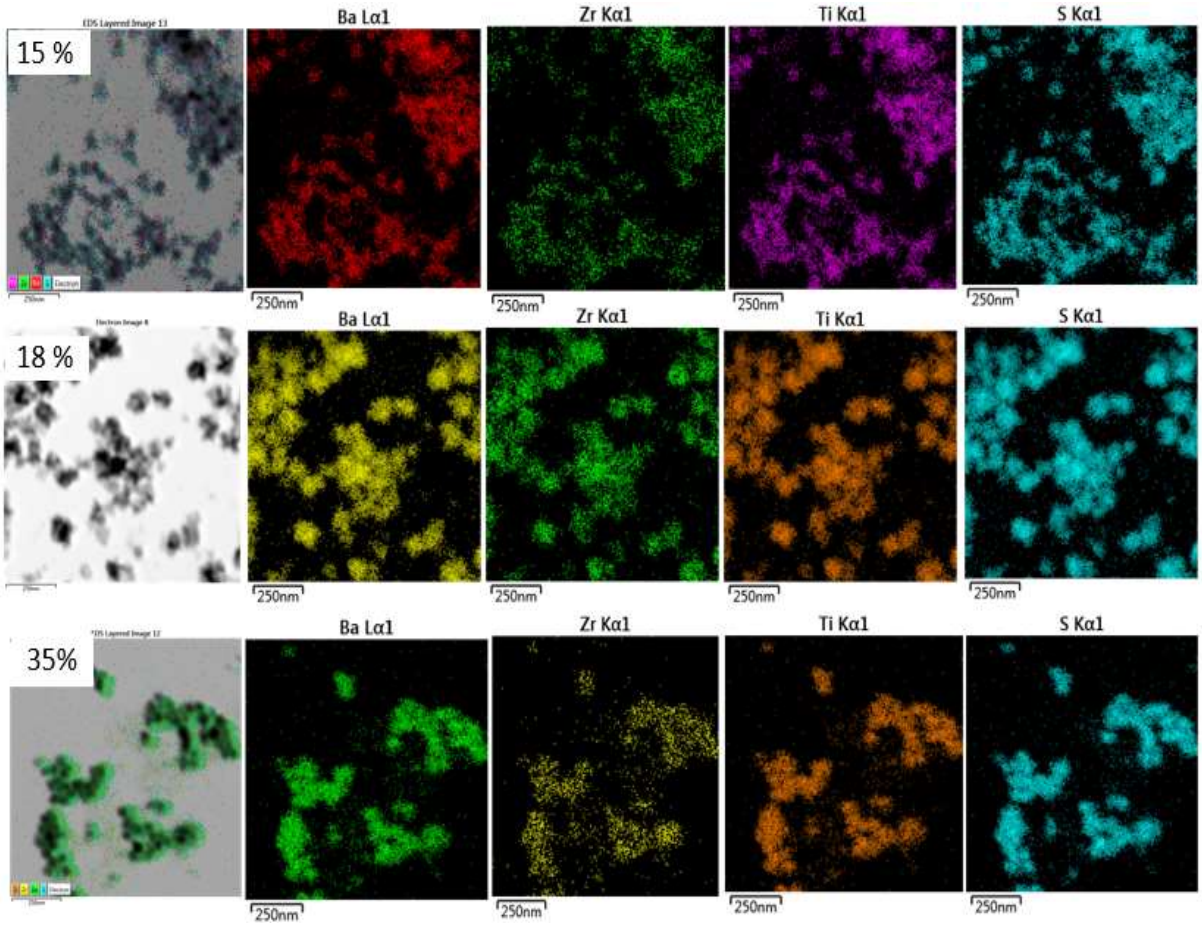

Figure S13. EDX mapping for $Ba(Zr_{1-x}Ti_x)S_3$ nanocrystal samples with 15-35% Ti content.

Table S2. Elemental composition from EDX data and calculated titanium percentages compared with the ICP data for samples with different compositions.

Atom %	**EDX composition**						
Ba %	26.5	24.9	30.2	28.9	27.2	25.1	29
Zr %	18.5	18.4	15.3	15.7	13.3	11.2	9
Ti %	0	1.2	1.9	2.4	4.1	7.2	11.2
S %	55	55.5	52.6	53	55.4	56.5	50.9
EDS (Ti/Zr+Ti) %	0	6	11	13	23	39	55
ICP (Ti/Zr+Ti) %	0	11	15	18	23	35	59
ICP Ba:Zr	1:1.05	1:1.12	1:0.89	1:0.84	1:0.81	1:0.70	1:0.44

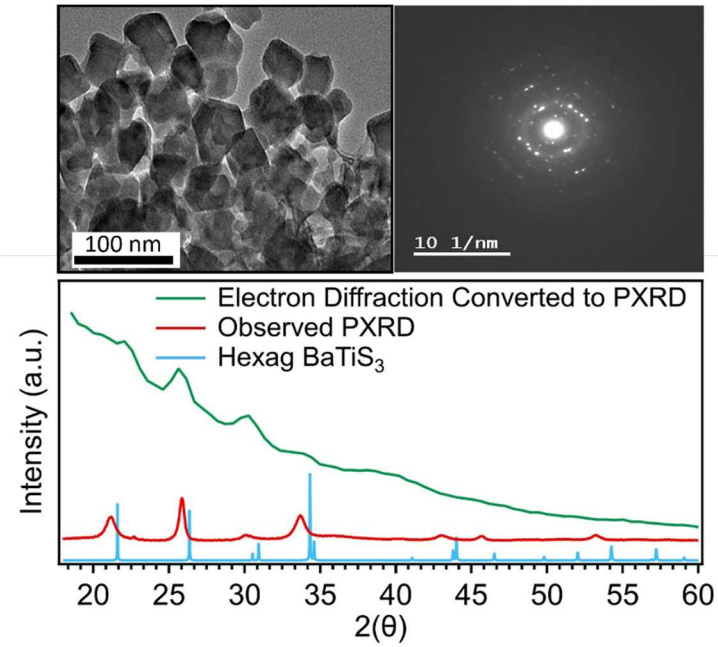

Figure S14. TEM image and electron diffraction data of 28% Ti alloyed $Ba(Zr_{1-x}Ti_x)S_3$ sample (top). The bottom panel compares the measured PXRD data for this sample to the integrated electron diffraction pattern, artificially converted to analogous Cu $K_{\alpha 1}$ diffraction data to facilitate comparison. Reference data for hexagonal $P6_3/mmc$ $BaTiS_3$ is also plotted.

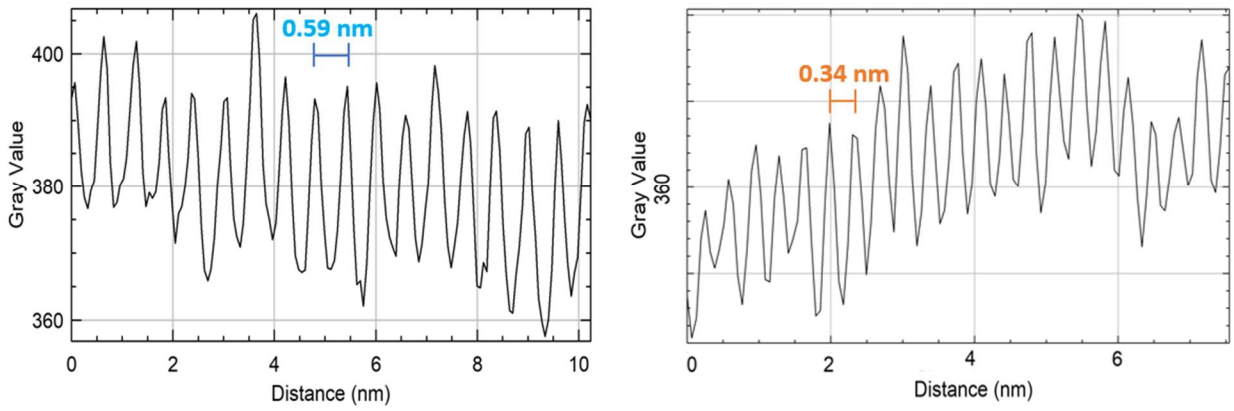

Figure S15. Intensity profiles of the regions highlighted by blue (left) and orange (right) boxes in Figure 6 of the main text, showing the 0.59 nm and 0.34 nm spacing, respectively, of the lattice fringes.

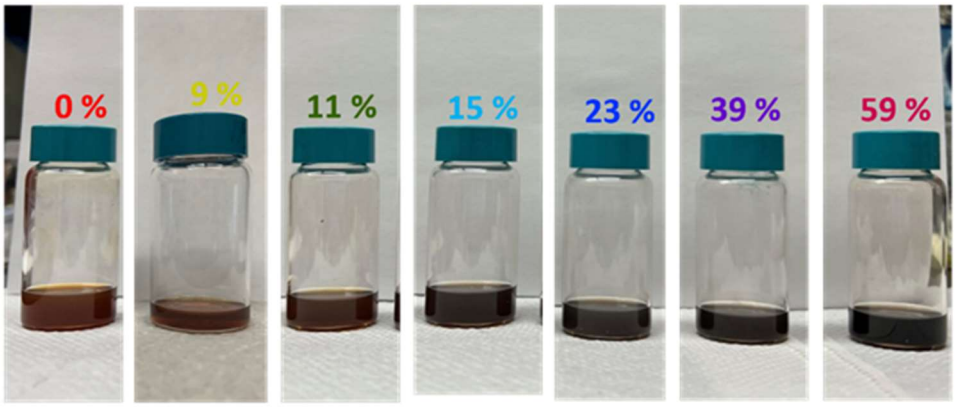

Figure S16. Photograph of $Ba(Zr_{1-x}Ti_x)S_3$ nanoparticles as suspensions in chloroform.

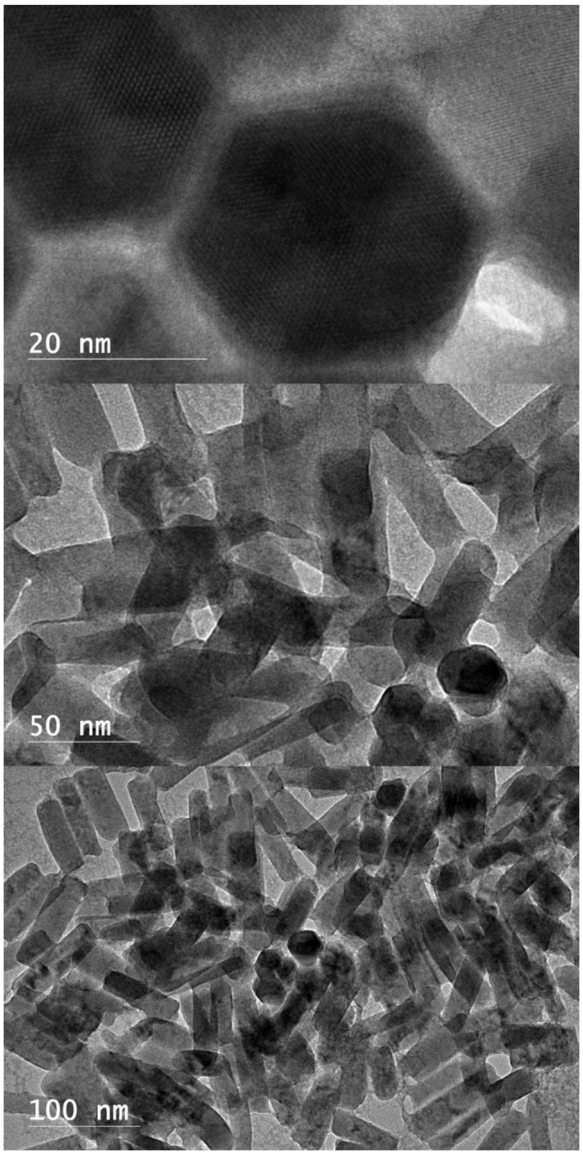

Figure S17. Additional TEM data for aliquots taken from a reaction after 10 minutes at 258 °C.

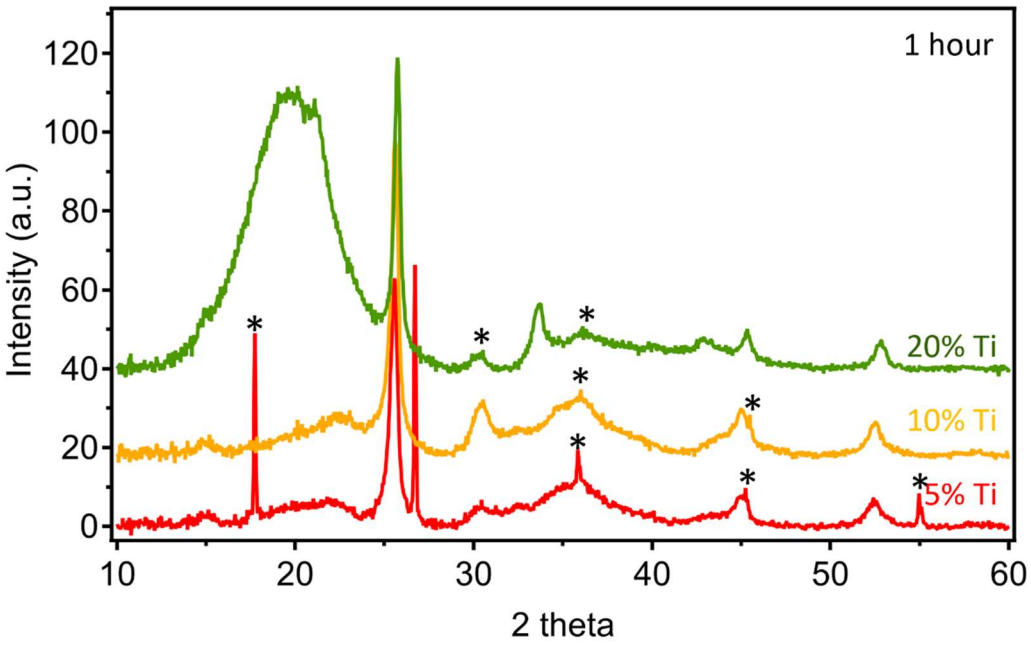

Figure S18. PXRD Data of samples synthesized using a 1 hour reaction time. Labeled titanium contents refer to nominal percentages. The identity of the impurity phase(s) seen in the 1-hour samples is not known (*).

X-Ray Photoelectron Spectroscopy (XPS) Analysis

XPS spectra were recorded on $Ba(Zr_{1-x}Ti_x)S_3$ films before and after being exposed to air for two weeks. The sample used for this measurement had 59% titanium content.

Before Aging (<1 day air exposure):

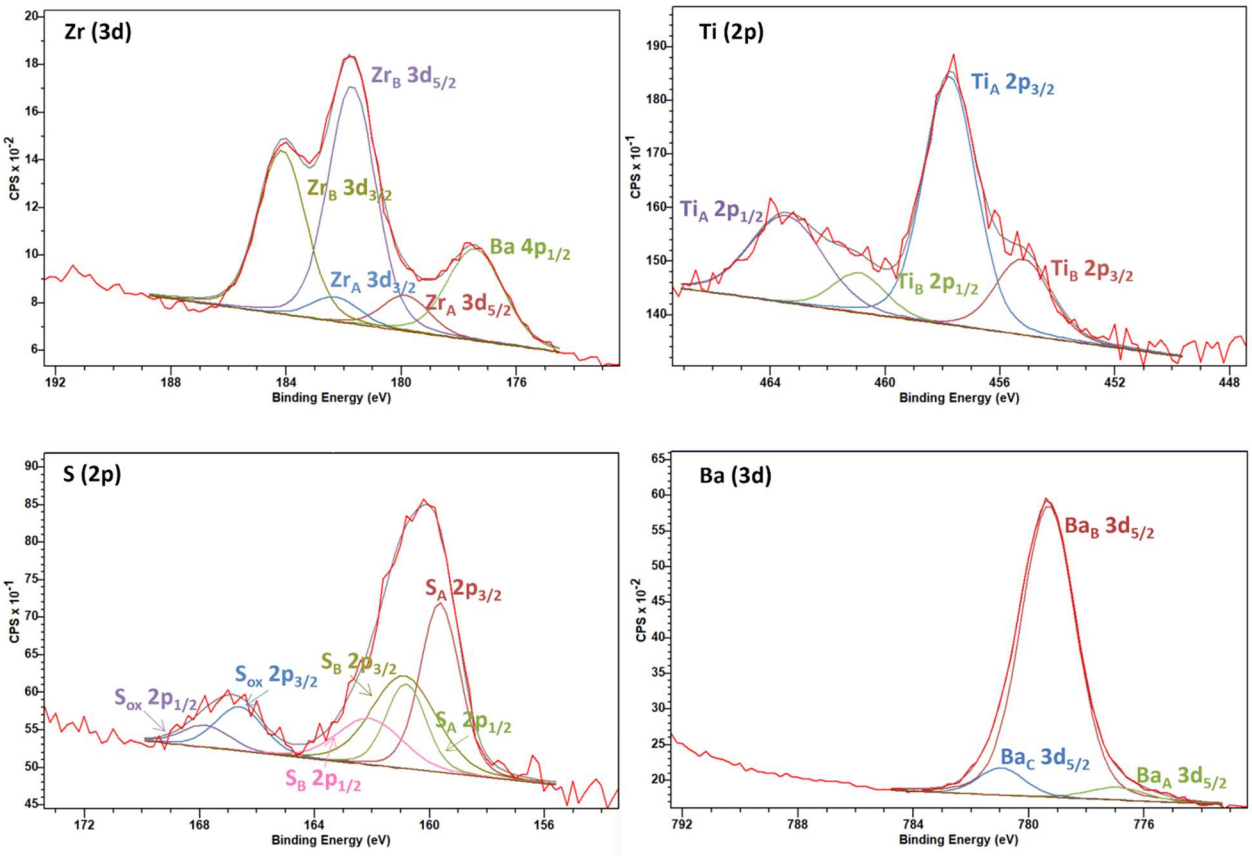

Figure S19. XPS spectra of 59% titanium-containing nanocrystals deposited as a drop-cast film on glass, after having been exposed to air for less than one day. The energy scale was calibrated by setting the C_{1s} peak to 285 eV. Fits were constrained by setting the Zr $3d_{5/2}$ and Zr $3d_{3/2}$ peaks to have the same FWHM, an intensity ratio of 0.688:1, and an energy difference of 2.43 eV; the Ti $2p_{3/2}$ and Ti $2p_{1/2}$ peaks were constrained to have an intensity ratio of 0.5:1 and an energy difference of 5.7 eV; and the S $2p_{3/2}$ and S $2p_{1/2}$ peaks were constrained to have an intensity ratio of 0.5:1, the same FWHM, and an energy difference of 1.18 eV.

After Aging (Two weeks of air exposure):

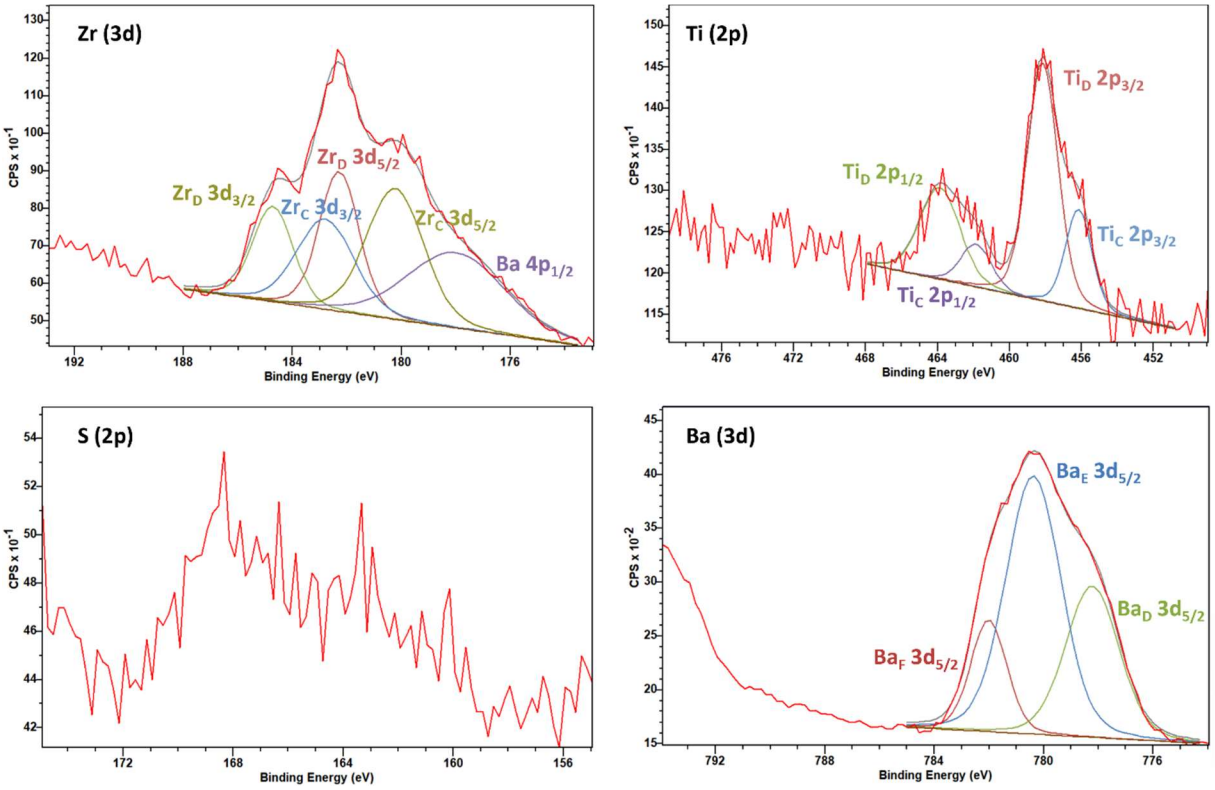

Figure S20. XPS spectra of 59% titanium-containing nanocrystals deposited as a drop-cast film on glass, after having been exposed to air for two weeks. Energy calibration and fitting was performed as described in the caption of Figure S19. Fitting of the sulfur regio was not attempted due to the low signal in this region.

Table S3 XPS Zr 3d Region Fitting Results

	Before Aging				After Aging			
	Zr $3d_{3/2}$ (eV)	Zr $3d_{5/2}$ (eV)	% of Zr species	Ba $4p_{3/2}$	Zr $3d_{3/2}$ (eV)	Zr $3d_{5/2}$ (eV)	% of Zr species	Ba $4p_{3/2}$
Zr_A	181.7	184.2	83%	177.4				178.0
Zr_B	179.9	182.28	13%					
Zr_C	--	--	--		182.29	184.72	42%	
Zr_D	--	--	--		180.24	182.79	58%	

Table S4 XPS Ti 2p Region Fitting Results

	Before Aging			After Aging		
	Ti $2p_{1/2}$ (eV)	Ti $2p_{3/2}$ (eV)	% of Ti species	Ti $2p_{1/2}$ (eV)	Ti $2p_{3/2}$ (eV)	% of Ti species
Ti_A	460.9	455.2	25%			
Ti_B	463.5	457.8	75%			
Ti_C	--	--	--	461.9	456.2	26%
Ti_D	--	--	--	463.9	458.2	74%

Table S5 XPS S 2p Region Fitting Results

	Before Aging			After Aging
	S $2p_{1/2}$ (eV)	S $2p_{3/2}$ (eV)	% of S species	
S_A	160.8	159.6	45%	Signal too low to fit
S_B	162.1	160.9	14%	
S_{ox}	167.8	166.6	40%	

Table S6 XPS Ba 3d Region Fitting Results

	Before Aging		After Aging	
	Ba $3d_{5/2}$ (eV)	% of Ba species	Ba $3d_{5/2}$ (eV)	% of Ba species
Ba_A	776.9	4	778.2	31
Ba_B	779.3	89	780.4	54
Ba_C	781.0	7	782.0	15

Computational Methods:

Calculations were carried out using the Quantum Espresso suit and the program PWSCF, version 7.2, using the frozen-core projector augmented-wave (PAW) method with the PBESOL functional. The cut-off kinetic energy for wavefunctions was 35 Ry and for the charge density the kinetic energy cut-off was 280 Ry. For geometry optimizations, atomic positions and lattice parameters were allowed to relax while maintaining the Bravais lattice of the structure; the BFGS quasi-newton algorithm was used for ion and cell dynamics. Sample complete input files are provided below for references.

For electronic property calculations (band gap and density of states), the GGA+U method was used with values of U_{eff} = 4.5 eV for Zr d-orbitals and U_{eff} = 4.0 eV for Ti d-orbitals.

Alloy calculations were carried out using supercells of the $BaTiS_3$ *P*6_3/mmc (hexagonal) and $BaZrS_3$ *P*nma (orthorhombic) structures. For the hexagonal case, a 2 x 2 x 2 supercell for the orthorhombic case, a 2 x 1 x 2 supercell was used; in both cases this supercell contains 80 atoms (16 formula units).

In alloyed structures, Zr and Ti were distributed over the octahedral B-sites. The program Supercell was used to generate all possible unique distributions of the ions for the cases of 1 Ti/15 Zr, 2 Ti/14 Zr, 4

Ti/12 Zr, and 8 Ti/8 Zr in each structure type (orthorhombic and hexagonal). For each alloy, a subset of the possible arrangements were subjected to geometry optimization; in each case, this was selected to include several high-symmetry arrangements (e.g., perfectly alternating for the 8 Ti/8 Zr case, or arrangements in chains and/or planes) and cases where the minority Ti ion were clustered (e.g. in pairs for the 2 Ti/14 Zr case) or as far as part as possible within the confines of the supercell. In addition to these deliberately selected cases, a few additional structures chosen at random were included. After optimization, the lowest energy structure was used for electronic property calculations unless otherwise stated.

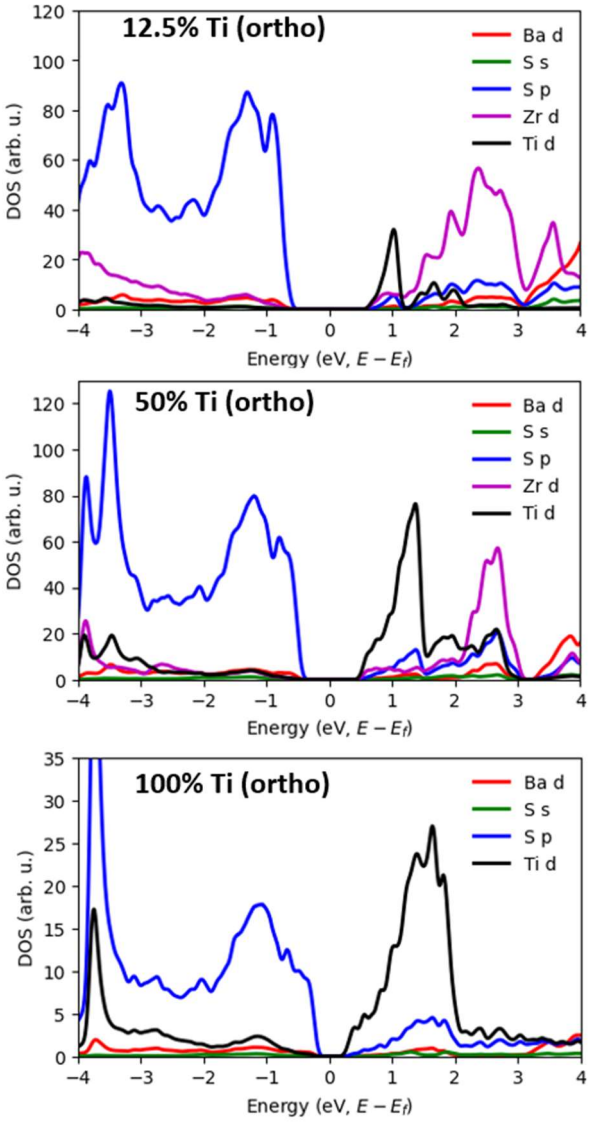

Figure S21. Partial DOS plots for orthorhombic structure at compositions not shown in main text (12.5 % Ti, 50% Ti, and 100% Ti). Note that the 100% Ti calculation was carried out for a single cell rather than a supercell, while the others were carried out on the standard 2 x 1 x 2 supercell. Energies are plotted relative to the Fermi level (E_f), which is set to the midpoint between the conduction band minimum and valence band maximum.

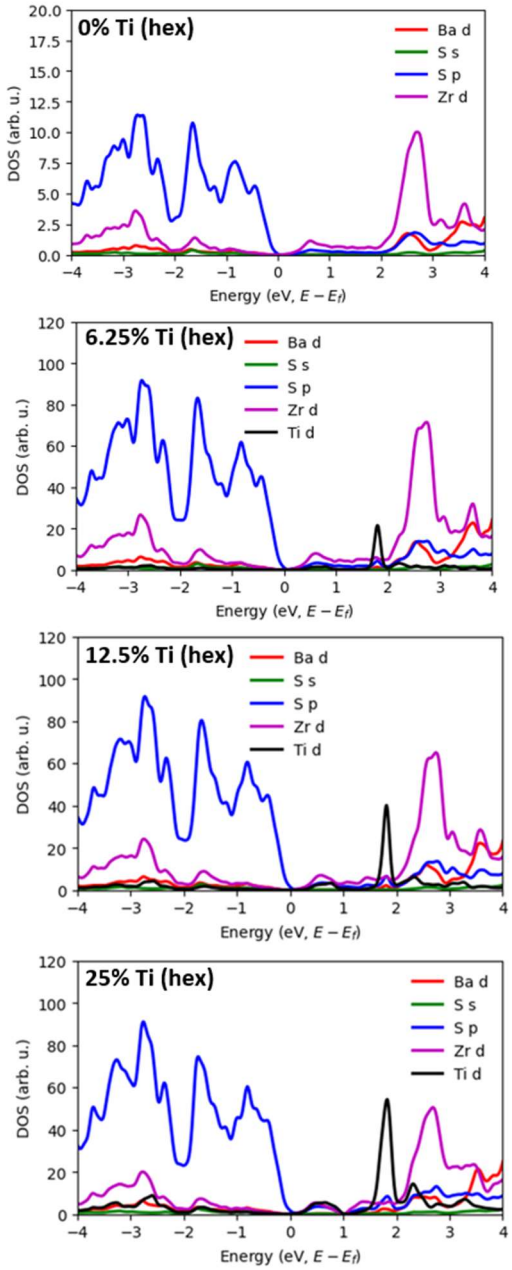

Figure S22. Partial DOS plots for $BaZr_xTi_{1-x}S_3$ in hexagonal polymorph with Ti content from 0 to 25%. Note that the 0% Ti case was calculated on a single unit cell; alloys were calculated using 2 x 2 x 2 supercell. Energies are plotted relative to the Fermi level (E_f), which is set to the midpoint between the conduction band minimum and valence band maximum.

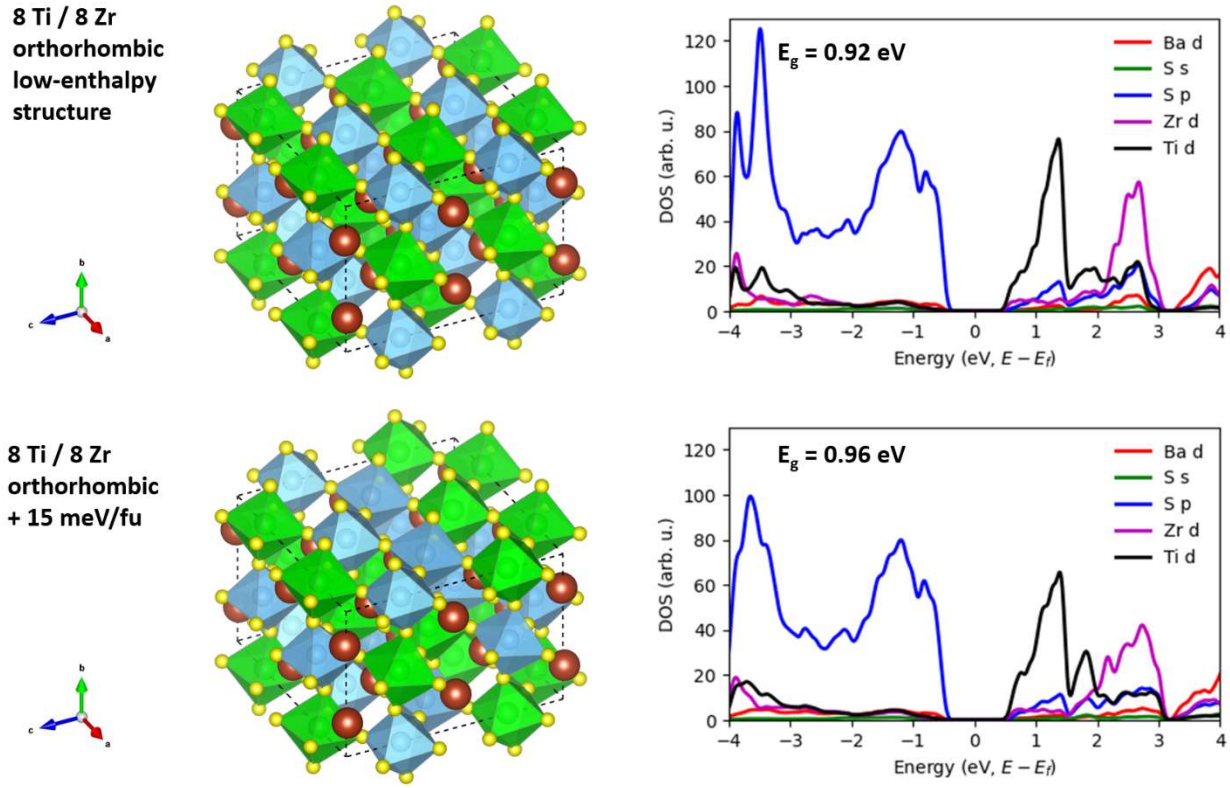

Figure S24. Compares two calculated structures for the 50% Ti in orthorhombic $BaZr_XTi_{1-x}S_3$ case, the lowest enthalpy structure with strictly alternating Ti/Zr ions and a higher enthalpy structure with Ti ions clustered into planes. Energies are plotted relative to the Fermi level (E_f), which is set to the midpoint between the conduction band minimum and valence band maximum.

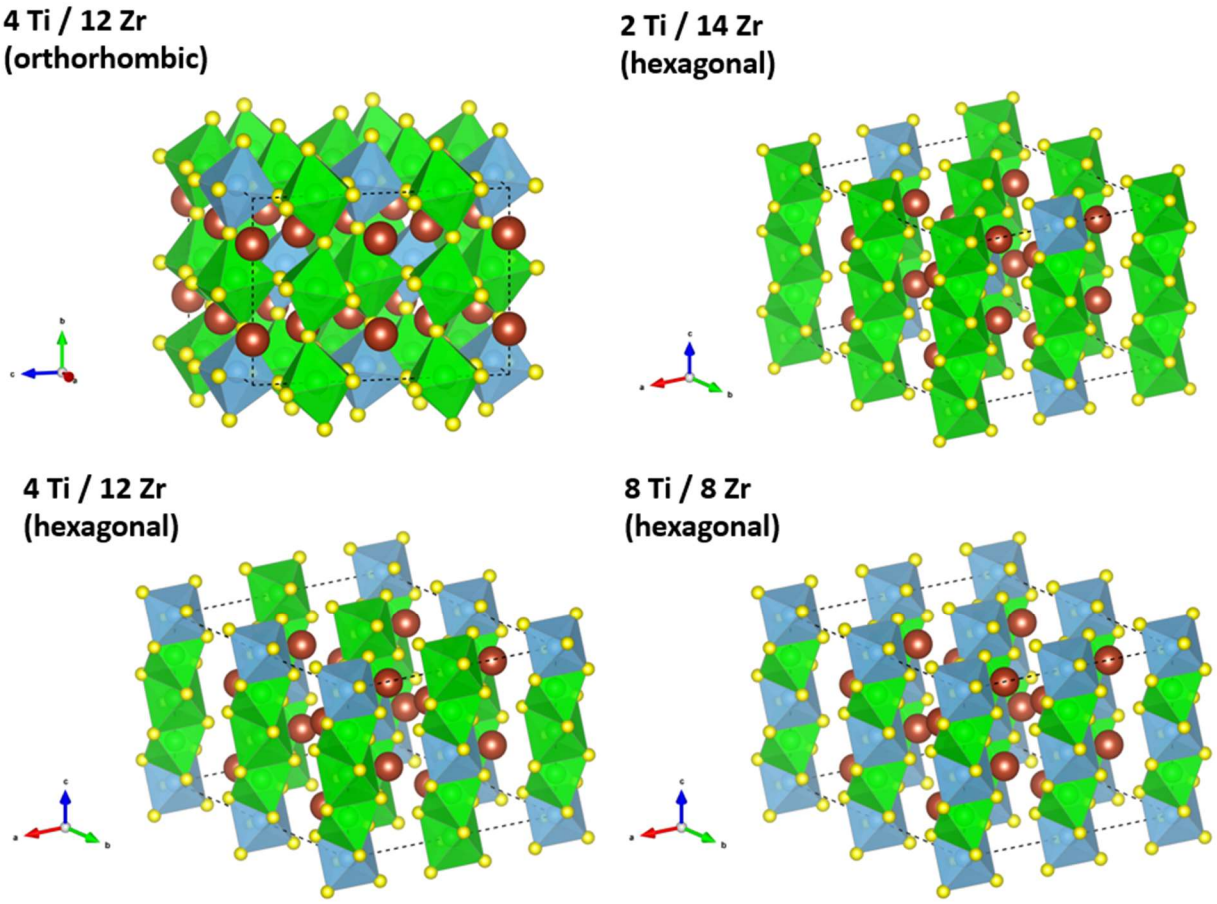

Figure S25. Depictions of low-enthalpy structures of other selected compositions of orthorhombic and hexagonal $BaZr_XTi_{1-x}S_3$.

Sample Input File for Structure Optimization for 2 X 1 X 2 orthorhombic supercell with 2 Ti Ions

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  tstress = .true.
  verbosity = 'high'
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  b = 9.9081600000
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  mixing_beta =   3.0000000000d-01
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/
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S      32.065 S.upf
Zr     91.224 Zr.upf
Ti     47.867 Ti.upf
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ATOMIC_POSITIONS crystal

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Ba	0.9812000000	0.7500000000	0.4965500000
Ba	0.5188000000	0.2500000000	0.0034500000
Ba	0.7312000000	0.7500000000	0.2534500000
Ba	0.7688000000	0.2500000000	0.2465500000
Ba	0.4812000000	0.7500000000	0.9965500000
Ba	0.5188000000	0.2500000000	0.5034500000
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S	0.5022500000	0.7500000000	0.7193000000
S	0.4977500000	0.2500000000	0.7807000000
S	0.7522500000	0.7500000000	0.0307000000
S	0.7477500000	0.2500000000	0.4693000000
S	0.5022500000	0.7500000000	0.2193000000
S	0.1077500000	0.9707000000	0.3934500000
S	0.1422500000	0.0293000000	0.6434500000
S	0.3577500000	0.5293000000	0.8565500000
S	0.8922500000	0.4707000000	0.6065500000
S	0.8922500000	0.0293000000	0.6065500000
S	0.3577500000	0.9707000000	0.8565500000
S	0.1422500000	0.4707000000	0.6434500000
S	0.1077500000	0.5293000000	0.3934500000
S	0.1077500000	0.9707000000	0.8934500000
S	0.1422500000	0.0293000000	0.1434500000
S	0.3577500000	0.5293000000	0.3565500000

S 0.8922500000 0.4707000000 0.1065500000
S 0.8922500000 0.0293000000 0.1065500000
S 0.3577500000 0.9707000000 0.3565500000
S 0.1422500000 0.4707000000 0.1434500000
S 0.1077500000 0.5293000000 0.8934500000
S 0.6077500000 0.9707000000 0.3934500000
S 0.6422500000 0.0293000000 0.6434500000
S 0.8577500000 0.5293000000 0.8565500000
S 0.3922500000 0.4707000000 0.6065500000
S 0.3922500000 0.0293000000 0.6065500000
S 0.8577500000 0.9707000000 0.8565500000
S 0.6422500000 0.4707000000 0.6434500000
S 0.6077500000 0.5293000000 0.3934500000
S 0.6077500000 0.9707000000 0.8934500000
S 0.6422500000 0.0293000000 0.1434500000
S 0.8577500000 0.5293000000 0.3565500000
S 0.3922500000 0.4707000000 0.1065500000
S 0.3922500000 0.0293000000 0.1065500000
S 0.8577500000 0.9707000000 0.3565500000
S 0.6422500000 0.4707000000 0.1434500000
S 0.6077500000 0.5293000000 0.8934500000
Zr 0.0000000000 0.0000000000 0.2500000000
Zr 0.2500000000 0.0000000000 0.5000000000
Zr 0.2500000000 0.5000000000 0.0000000000
Zr 0.0000000000 0.5000000000 0.7500000000
Zr 0.0000000000 0.0000000000 0.7500000000
Zr 0.2500000000 0.0000000000 0.0000000000
Zr 0.2500000000 0.5000000000 0.5000000000
Ti 0.0000000000 0.5000000000 0.2500000000
Zr 0.5000000000 0.0000000000 0.2500000000
Zr 0.7500000000 0.0000000000 0.5000000000
Zr 0.7500000000 0.5000000000 0.0000000000
Zr 0.5000000000 0.5000000000 0.7500000000
Ti 0.5000000000 0.0000000000 0.7500000000
Zr 0.7500000000 0.0000000000 0.0000000000
Zr 0.7500000000 0.5000000000 0.5000000000
Zr 0.5000000000 0.5000000000 0.2500000000
K_POINTS automatic
3 4 3 0 0 0

Sample Input File for Single-Point DFT+U Calculation Used for DOS and PDOS Calculations

```
&CONTROL
  calculation = 'scf'
  etot_conv_thr =   8.0000000000d-04
  forc_conv_thr =   1.0000000000d-03
  outdir = './out/'
  prefix = 'bazrs3_paw_pbesol_212_supercell_twoTi_006_scf'
  pseudo_dir = './paw-sr-11_pbesol_standard_upf'
  tprnfor = .true.
  tstress = .true.
  verbosity = 'high'
/
&SYSTEM
  ecutrho =   2.8000000000d+02
  ecutwfc =   3.5000000d+01
  ibrav = 8
 celldm(1) =     26.48041487
 celldm(2) =      0.70419828
 celldm(3) =      0.99160753
  nat = 80
  nosym = .false.
  ntyp = 4
  occupations = 'fixed'
/
&ELECTRONS
  conv_thr =   1.0000000000d-08
  electron_maxstep = 200
  mixing_beta =   3.0000000000d-01
  mixing_ndim = 12
/
ATOMIC_SPECIES
Ba     137.327 Ba.upf
S      32.065 S.upf
Zr     91.224 Zr.upf
Ti     47.867 Ti.upf

ATOMIC_POSITIONS crystal
Ba          0.0188000000      0.2500000000      0.0034500000
Ba          0.2312000000      0.7500000000      0.2534500000
Ba          0.2688000000      0.2500000000      0.2465500000
Ba          0.9812000000      0.7500000000      0.9965500000
Ba          0.0188000000      0.2500000000      0.5034500000
Ba          0.2312000000      0.7500000000      0.7534500000
```

Ba	0.2688000000	0.2500000000	0.7465500000
Ba	0.9812000000	0.7500000000	0.4965500000
Ba	0.5188000000	0.2500000000	0.0034500000
Ba	0.7312000000	0.7500000000	0.2534500000
Ba	0.7688000000	0.2500000000	0.2465500000
Ba	0.4812000000	0.7500000000	0.9965500000
Ba	0.5188000000	0.2500000000	0.5034500000
Ba	0.7312000000	0.7500000000	0.7534500000
Ba	0.7688000000	0.2500000000	0.7465500000
Ba	0.4812000000	0.7500000000	0.4965500000
S	0.9977500000	0.2500000000	0.2807000000
S	0.2522500000	0.7500000000	0.5307000000
S	0.2477500000	0.2500000000	0.9693000000
S	0.0022500000	0.7500000000	0.7193000000
S	0.9977500000	0.2500000000	0.7807000000
S	0.2522500000	0.7500000000	0.0307000000
S	0.2477500000	0.2500000000	0.4693000000
S	0.0022500000	0.7500000000	0.2193000000
S	0.4977500000	0.2500000000	0.2807000000
S	0.7522500000	0.7500000000	0.5307000000
S	0.7477500000	0.2500000000	0.9693000000
S	0.5022500000	0.7500000000	0.7193000000
S	0.4977500000	0.2500000000	0.7807000000
S	0.7522500000	0.7500000000	0.0307000000
S	0.7477500000	0.2500000000	0.4693000000
S	0.5022500000	0.7500000000	0.2193000000
S	0.1077500000	0.9707000000	0.3934500000
S	0.1422500000	0.0293000000	0.6434500000
S	0.3577500000	0.5293000000	0.8565500000
S	0.8922500000	0.4707000000	0.6065500000
S	0.8922500000	0.0293000000	0.6065500000
S	0.3577500000	0.9707000000	0.8565500000
S	0.1422500000	0.4707000000	0.6434500000
S	0.1077500000	0.5293000000	0.3934500000
S	0.1077500000	0.9707000000	0.8934500000
S	0.1422500000	0.0293000000	0.1434500000
S	0.3577500000	0.5293000000	0.3565500000
S	0.8922500000	0.4707000000	0.1065500000
S	0.8922500000	0.0293000000	0.1065500000
S	0.3577500000	0.9707000000	0.3565500000
S	0.1422500000	0.4707000000	0.1434500000
S	0.1077500000	0.5293000000	0.8934500000
S	0.6077500000	0.9707000000	0.3934500000
S	0.6422500000	0.0293000000	0.6434500000

S 0.8577500000 0.5293000000 0.8565500000
S 0.3922500000 0.4707000000 0.6065500000
S 0.3922500000 0.0293000000 0.6065500000
S 0.8577500000 0.9707000000 0.8565500000
S 0.6422500000 0.4707000000 0.6434500000
S 0.6077500000 0.5293000000 0.3934500000
S 0.6077500000 0.9707000000 0.8934500000
S 0.6422500000 0.0293000000 0.1434500000
S 0.8577500000 0.5293000000 0.3565500000
S 0.3922500000 0.4707000000 0.1065500000
S 0.3922500000 0.0293000000 0.1065500000
S 0.8577500000 0.9707000000 0.3565500000
S 0.6422500000 0.4707000000 0.1434500000
S 0.6077500000 0.5293000000 0.8934500000
Zr 0.0000000000 0.0000000000 0.2500000000
Zr 0.2500000000 0.0000000000 0.5000000000
Zr 0.2500000000 0.5000000000 0.0000000000
Zr 0.0000000000 0.5000000000 0.7500000000
Zr 0.0000000000 0.0000000000 0.7500000000
Zr 0.2500000000 0.0000000000 0.0000000000
Zr 0.2500000000 0.5000000000 0.5000000000
Ti 0.0000000000 0.5000000000 0.2500000000
Zr 0.5000000000 0.0000000000 0.2500000000
Zr 0.7500000000 0.0000000000 0.5000000000
Zr 0.7500000000 0.5000000000 0.0000000000
Zr 0.5000000000 0.5000000000 0.7500000000
Ti 0.5000000000 0.0000000000 0.7500000000
Zr 0.7500000000 0.0000000000 0.0000000000
Zr 0.7500000000 0.5000000000 0.5000000000
Zr 0.5000000000 0.5000000000 0.2500000000
K_POINTS automatic
3 4 3 0 0 0
HUBBARD (ortho-atomic)
U Zr-4d 4.5
U Ti-3d 4