Supporting information for: Band-gap engineering in $AB(O_xS_{1-x})_3$ perovskite oxysulfides: A route to strongly polar materials for photocatalytic water splitting

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S1. TOTAL ENERGIES OF STRAINED $BaZrS_3$

For $BaZrS_3$ we calculated the total energy as a function of strain for the experimental phase (non polar) and several polar phases (polarisation along the out-of-plane axis) with different rotation patterns. Figure S1 shows the energies of the non-polar and the energetically most stable polar phase. For compressive strains below 5%, the polar phase relaxes to a non-polar structure.

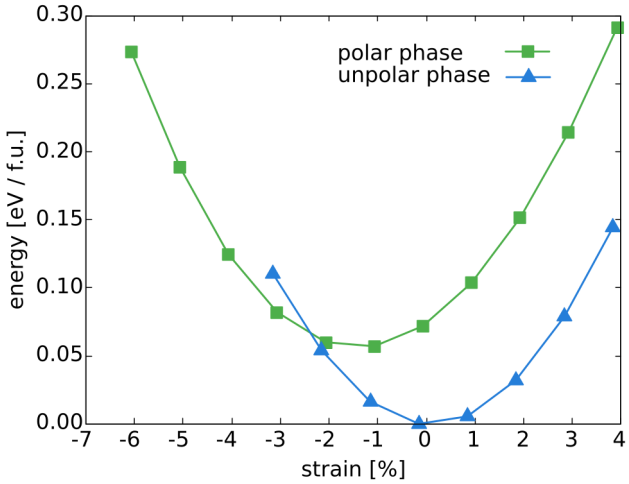

FIG. S1: Total energy as a function of the in-plane lattice parameter for the polar and non-polar phase.

S2. THERMODYNAMICAL STABILITY

To assess the thermodynamic stability the decomposition energy with respect to different decomposition products was calculated for $BaZrX_2Y$ (with X and Y being either oxygen or sulfur) as follows:

$$E_d(B) = min\{E_{tot}(BaX_2) + E_{tot}(ZrY), E_{tot}(BaY) + E_{tot}(ZrX_2)\} - E_{tot}(BaZrX_2Y) \quad (1)$$

$$E_d(T) = \big(2E_{tot}(BaZrX_3) + E_{tot}(BaZrY_3) - 3E_{tot}(BaZrX_2Y)\big)/3 \quad (2)$$

$$E_d(B+T) = \Big(min\{2E_{tot}(BaZrX_3) + E_{tot}(BaY) + E_{tot}(ZrY_2), \\ 2E_{tot}(BaZrX_3) + E_{tot}(BaY_2) + E_{tot}(ZrY)\} - 3E_{tot}(BaZrX_2Y)\Big)/3 \quad (3)$$

For $BaZr_yTi_{1-y}O_2$ we calculated the thermodynamical stability only with respect to ternary perovskite phases:

$$E_d(T) = \Big((1-y)\big(2E_{tot}(BaTiO_3) + E_{tot}(BaTiS_3)\big) + y\big(2E_{tot}(BaZrO_3) + E_{tot}(BaZrS_3)\big) - 3E_{tot}(BaZr_yTi_{1-y}O_2) \Big)/3 \quad (4)$$

S3. STRUCTURES

In tables I to X we give the atomic coordinates of the most important structures discussed in this work. For unstrained calculations all lattice parameters and all atomic coordinates were relaxed with the PBE+U functional; for the strained calculations the out-of-plane lattice parameter as well as all atomic coordinates were relaxed. Lattice parameters are given in Å and atomic positions in fractional coordinates (f.c.). VASP structure files have also been uploaded as supporting information.

TABLE I: Unstrained non-polar $BaZrS_3$

lattice parameter	x [Å]	y [Å]	z [Å]
a	9.99787499	-0.00000018	0.10557637
b	-0.00000015	9.98490675	0.00000084
c	0.15497803	0.00000081	9.99723137
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.75000007	0.50000007	0.24999950
Zr	0.24999991	-0.00000010	0.24999956
Zr	0.74999999	-0.00000005	0.24999959
Zr	0.24999991	0.50000006	0.24999968
Zr	0.75000009	0.49999994	0.75000032
Zr	0.25000001	0.00000005	0.75000041
Zr	0.75000009	0.00000010	0.75000044
Zr	0.24999993	0.49999993	0.75000050
S	0.20503574	0.53891900	0.00037474
S	0.20503578	0.96108107	0.00037538
S	0.50037536	0.53891896	0.20503547
S	0.50037471	0.96108111	0.20503552
S	0.28159628	0.24999964	0.20736353
S	0.79263634	0.74999967	0.21840283
S	0.70736399	0.25000033	0.28159594
S	0.21840321	0.75000035	0.29263586
S	0.99962454	0.46108114	0.29496353
S	0.99962519	0.03891880	0.29496362
S	0.29496378	0.03891871	0.49962471
S	0.29496381	0.46108124	0.49962544
S	0.70503619	0.53891876	0.50037456
S	0.70503622	0.96108129	0.50037528
S	0.00037481	0.96108120	0.70503638
S	0.00037547	0.53891886	0.70503646
S	0.78159679	0.24999965	0.70736414
S	0.29263601	0.74999967	0.71840406
S	0.20736366	0.25000033	0.78159717
S	0.71840372	0.75000036	0.79263647
S	0.49962529	0.03891889	0.79496448
S	0.49962464	0.46108104	0.79496453
S	0.79496422	0.03891893	0.99962462
S	0.79496426	0.46108100	0.99962526
Ba	0.53631773	0.24999984	0.02272570
Ba	0.02272575	0.24999994	0.03631806
Ba	0.47727435	0.75000011	0.46368202
Ba	0.96368189	0.75000013	0.47727419
Ba	0.03631811	0.24999986	0.52272578
Ba	0.52272565	0.24999989	0.53631798
Ba	0.97727426	0.75000006	0.96368194
Ba	0.46368227	0.75000016	0.97727430

TABLE II: Polar -5% strained (in the ac plane) $BaZrS_3$

lattice parameter	x [Å]	y [Å]	z [Å]
a	9.48459182	0.00000000	0.00000000
b	0.00000059	10.50831545	-0.00003643
c	0.00000000	0.00000000	9.48459182
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.24999899	0.25814548	0.25001016
Zr	0.75000033	0.25814929	0.25001021
Zr	0.75000055	0.75814903	0.25001076
Zr	0.24999901	0.75814511	0.25001081
Zr	0.24999893	0.75814504	0.75001178
Zr	0.75000043	0.75814915	0.75001185
Zr	0.24999906	0.25814537	0.75001211
Zr	0.75000044	0.25814933	0.75001220
S	0.32750048	0.25243057	0.00001112
S	0.17249928	0.75243010	0.00001123
S	-0.00000036	0.25243224	0.17250931
S	0.49999984	0.75243343	0.17251291
S	0.74999893	0.50374951	0.25000777
S	0.25000042	0.50374824	0.25000798
S	0.24999313	1.00374809	0.25000958
S	0.75000615	0.00374943	0.25000973
S	0.49999972	0.25242895	0.32750752
S	-0.00000031	0.75242696	0.32751072
S	0.17250185	0.25243152	0.50001109
S	0.82749691	0.25243233	0.50001114
S	0.67250309	0.75243183	0.50001124
S	0.32749722	0.75243109	0.50001128
S	-0.00000036	0.75243197	0.67251070
S	0.49999981	0.25243376	0.67251345
S	0.74999974	0.00374937	0.75001381
S	0.24999959	1.00374797	0.75001381
S	0.24999404	0.50374825	0.75001530
S	0.75000530	0.50374954	0.75001569
S	0.49999975	0.75242864	0.82750854
S	-0.00000031	0.25242727	0.82751206
S	0.67249971	0.25243112	1.00001113
S	0.82749975	0.75243128	1.00001124
Ba	0.50000029	1.00322217	0.00001210
Ba	0.49999944	0.50322327	0.00001285
Ba	0.50000031	0.50322333	0.50001200
Ba	0.99999902	0.00322262	0.50001206
Ba	0.49999939	1.00322345	0.50001271
Ba	0.99999990	0.50322214	0.50001298
Ba	0.99999896	0.50322241	1.00001206
Ba	1.00000019	0.00322101	1.00001303

TABLE III: unstrained *trans* $BaZrO_2S$

lattice parameter	x [Å]	y [Å]	z [Å]
a	8.12283552	0.00022342	-0.08917423
b	-0.00022459	8.12333213	-0.00047672
c	0.13063233	0.00070326	11.90389813
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.24998242	0.24998811	0.00995679
Zr	0.74998375	0.24998743	0.00995682
Zr	0.74998264	0.74998817	0.00995683
Zr	0.24998350	0.74998752	0.00995693
Zr	0.75000576	0.75001289	0.50995760
Zr	0.25000785	0.75001135	0.50995762
Zr	0.25000589	0.25001276	0.50995765
Zr	0.75000772	0.25001123	0.50995772
S	0.25006398	0.25000734	0.21513651
S	0.75005434	0.24999731	0.21513653
S	0.75006452	0.75000777	0.21513653
S	0.25005381	0.74999774	0.21513669
S	0.75005941	0.75000669	0.71513567
S	0.25005292	0.74999293	0.71513569
S	0.25005960	0.25000616	0.71513570
S	0.75005273	0.24999239	0.71513581
Ba	0.50004829	0.50001279	0.32007459
Ba	0.50003864	0.00001234	0.32007467
Ba	0.00004827	0.00001292	0.32007490
Ba	0.00003865	0.50001227	0.32007492
Ba	1.00002464	0.99998116	0.82007632
Ba	1.00000692	0.49998856	0.82007642
Ba	0.50002462	0.49998121	0.82007647
Ba	0.50000690	0.99998846	0.82007659
O	0.99996034	0.25000063	-0.03758397
O	0.49996028	0.75000074	-0.03758375
O	0.74994715	0.99998899	-0.03756274
O	0.24994653	0.49998904	-0.03756264
O	0.49998141	0.75000022	0.46240290
O	0.99998138	0.24999955	0.46240321
O	0.74995208	0.50001092	0.46241239
O	0.24995214	0.00001095	0.46241248
O	0.49998170	0.25000512	0.46242081
O	-0.00001833	0.75000555	0.46242096
O	0.24994545	0.50001067	0.46242547
O	0.74994525	1.00001072	0.46242557
O	0.24994248	-0.00001063	0.96239964
O	0.74994295	0.49998942	0.96239980
O	-0.00003924	0.74999528	0.96240963
O	0.49996072	0.24999507	0.96240978

TABLE IV: unstrained *cis* $BaZrO_2S$

lattice parameter	x [Å]	y [Å]	z [Å]
a	9.35569399	0.02726452	-0.09592231
b	0.02741990	8.17287188	-0.02939200
c	0.15327688	-0.02574557	9.35518125
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.22771608	0.23859581	0.23136184
Zr	0.72771200	0.73847232	0.23137562
Zr	0.27259105	0.73864507	0.27621391
Zr	0.77258592	0.23853464	0.27629553
Zr	0.22763376	0.73856740	0.73138261
Zr	0.72758738	0.23851969	0.73139969
Zr	0.77253603	0.73848382	0.77627909
Zr	0.27253209	0.23854257	0.77629665
S	0.28129405	0.78445404	0.01124908
S	-0.00731856	0.78436746	0.22263980
S	0.49268739	0.28427938	0.22267037
S	0.78134282	0.78434432	0.51129939
S	0.28137828	0.28426910	0.51130990
S	-0.00744726	0.28443371	0.72263434
S	0.49261355	0.78435528	0.72271325
S	0.78129148	0.28447292	1.01130985
Ba	0.50569721	0.50657404	-0.04053781
Ba	0.54458246	1.00651894	-0.00184653
Ba	1.00589160	0.50659109	0.45939332
Ba	0.50583942	1.00649327	0.45944583
Ba	0.54450556	0.50657822	0.49810133
Ba	1.04455217	0.00657185	0.49812036
Ba	1.00567287	0.00662105	0.95942905
Ba	1.04452926	0.50659616	0.99815368
O	0.21158844	0.22747964	0.01031970
O	0.70440154	-0.00454999	0.24502901
O	0.20435664	0.49549644	0.24503345
O	0.49370552	0.72741053	0.29220176
O	-0.00631585	0.22740373	0.29233998
O	0.25897183	0.99546415	0.29968052
O	0.75898816	0.49543324	0.29979499
O	0.21172370	0.72747663	0.51030548
O	0.71154964	0.22732480	0.51034449
O	0.70412505	0.49540671	0.74502272
O	0.20413438	0.99548414	0.74505030
O	-0.00639029	0.72732267	0.79230113
O	0.49358839	0.22729299	0.79243277
O	0.25891264	0.49545235	0.79968916
O	0.75892477	-0.00458860	0.79975966
O	0.71172885	0.72731292	1.01030472

TABLE V: unstrained *trans* $BaZrOS_2$

lattice parameter	x [Å]	y [Å]	z [Å]
a	10.29508773	-0.00015358	-0.11699885
b	0.00030355	10.11902845	0.00012494
c	0.09399252	0.00017589	8.14883175
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.24925453	0.25042821	0.25458719
Zr	0.74928442	0.25050460	0.25466202
Zr	0.24935374	0.75037482	0.25473706
Zr	0.74933644	0.75052013	0.25476167
Zr	0.24926328	0.25037999	0.75461266
Zr	0.74925218	0.25058140	0.75464169
Zr	0.74932242	0.75054683	0.75472094
Zr	0.24933430	0.75037337	0.75473970
S	0.24931286	0.50038523	0.20550184
S	0.74935685	0.00051313	0.20550804
S	0.49927319	0.25042246	0.25451338
S	-0.00073416	0.25045673	0.25466505
S	0.49935375	0.75042950	0.25474484
S	-0.00062829	0.75045709	0.25476163
S	0.24932409	1.00038469	0.30369229
S	0.74930204	0.50053094	0.30378883
S	0.24912871	1.00036932	0.70548977
S	0.74908415	0.50057582	0.70553477
S	-0.00077421	0.25059966	0.75461683
S	0.49934778	0.75057917	0.75466949
S	-0.00063676	0.75033785	0.75469425
S	0.49923629	0.25033256	0.75477174
S	0.74943954	0.00057789	0.80369590
S	0.24940321	0.50035450	0.80382709
Ba	0.45589191	1.00037252	0.00463512
Ba	0.54277385	0.50042385	0.00471755
Ba	1.04281071	0.50030410	0.50464038
Ba	0.95588298	0.00041288	0.50465768
Ba	0.54280896	1.00054145	0.50466527
Ba	0.45575922	0.50049314	0.50473592
Ba	0.95573151	0.50061220	1.00456930
Ba	1.04267805	0.00055308	1.00465730
O	0.24912629	0.20566874	0.00461438
O	0.24944483	0.79492331	0.00462708
O	0.24925700	0.29508084	0.50460650
O	0.74913285	0.20594803	0.50463889
O	0.24947748	0.70553374	0.50464386
O	0.74941693	0.79531116	0.50465369
O	0.74918246	0.29534251	1.00463705
O	0.74943463	0.70596708	1.00466136

TABLE VI: unstrained *cis* $BaZrOS_2$

lattice parameter	x [Å]	y [Å]	z [Å]
a	9.06276968	-0.03115744	-0.02779567
b	-0.02852555	10.34021075	0.02922366
c	0.19849010	0.03117037	9.06064787
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.23103535	0.74912920	0.22609694
Zr	0.73103033	0.24913367	0.22611566
Zr	0.77786335	0.74912652	0.27292347
Zr	0.27784082	0.24913622	0.27292681
Zr	0.73103441	0.74912510	0.72609362
Zr	0.23102843	0.24913414	0.72611313
Zr	0.27786044	0.74912740	0.77292212
Zr	0.77784463	0.24913133	0.77292788
S	0.19235535	0.23515263	0.00574536
S	0.72987199	0.00484108	0.22436796
S	0.22984261	0.50484469	0.22437182
S	0.27958058	1.00484724	0.27408448
S	0.77959053	0.50483815	0.27412985
S	0.49823430	0.73514112	0.31151414
S	-0.00178903	0.23514897	0.31160088
S	0.19244497	0.73515088	0.50572484
S	0.69236270	0.23511836	0.50574607
S	0.72983361	0.50483398	0.72435786
S	0.22985029	1.00484270	0.72437887
S	0.77959264	0.00483642	0.77410268
S	0.27959733	0.50483995	0.77410363
S	-0.00176675	0.73512018	0.81150884
S	0.49821208	0.23511640	0.81159614
S	0.69245032	0.73510970	1.00572389
Ba	0.48872805	0.97519444	-0.01004803
Ba	0.51400906	0.47522166	0.01526227
Ba	0.48869150	0.47523141	0.48992812
Ba	0.98870265	-0.02476977	0.48994922
Ba	0.51399092	0.97521709	0.51524760
Ba	1.01401931	0.47525581	0.51528407
Ba	0.98867655	0.47524642	0.98995341
Ba	1.01401974	-0.02478646	1.01524138
O	0.28003511	0.78797759	0.00264185
O	0.00131663	0.78797311	0.22391543
O	0.50129777	0.28799547	0.22393748
O	0.78004375	0.78797229	0.50264215
O	0.28003108	0.28798580	0.50265889
O	0.00129775	0.28798748	0.72392450
O	0.50131624	0.78798293	0.72392529
O	0.78002263	0.28799322	1.00265944

TABLE VII: unstrained $BaZrO_3$

lattice parameter	x [Å]	y [Å]	z [Å]
a	8.37255246	-0.00772348	-0.00616917
b	-0.00788601	8.39747648	-0.00639123
c	-0.00618204	-0.00624901	8.35459129
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.00000000	0.00000000	0.00000000
Zr	-0.00000000	0.50000000	0.00000000
Zr	0.50000000	-0.00000000	0.00000000
Zr	0.50000000	0.50000000	0.00000000
Zr	0.00000000	0.00000000	0.50000000
Zr	0.00000000	0.50000000	0.50000000
Zr	0.50000000	-0.00000000	0.50000000
Zr	0.50000000	0.50000000	0.50000000
O	0.48436124	0.75000403	0.02445374
O	0.98436143	0.25000403	0.02445459
O	0.25000932	0.48469955	0.03235989
O	0.75000935	0.98469943	0.03236013
O	0.46820045	0.02352152	0.24999462
O	0.96820087	0.52352228	0.24999462
O	0.03179900	0.97647724	0.25000543
O	0.53179917	0.47647801	0.25000544
O	0.74999071	0.01530219	0.46763926
O	0.24999068	0.51530226	0.46763937
O	0.01564055	0.24999600	0.47554542
O	0.51564047	0.74999600	0.47554611
O	0.48435953	0.25000400	0.52445389
O	0.98435945	0.75000400	0.52445458
O	0.75000932	0.48469774	0.53236063
O	0.25000929	0.98469781	0.53236074
O	0.46820089	0.52352199	0.74999456
O	0.96820101	0.02352276	0.74999457
O	0.03179913	0.47647772	0.75000538
O	0.53179961	0.97647848	0.75000538
O	0.24999065	0.01530057	0.96763981
O	0.74999068	0.51530045	0.96764005
O	0.01563857	0.74999597	0.97554540
O	0.51563877	0.24999597	0.97554626
Ba	0.25107731	0.74937715	0.24960487
Ba	0.75107729	0.24937737	0.24960488
Ba	0.24892346	0.25062327	0.25039470
Ba	0.74892352	0.75062346	0.25039499
Ba	0.25107648	0.24937654	0.74960501
Ba	0.75107654	0.74937673	0.74960530
Ba	0.24892271	0.75062263	0.75039512
Ba	0.74892269	0.25062285	0.75039513

TABLE VIII: -2.5% strained (in the ab plane) $BaZr_{0.625}Ti_{0.375}O_2S$ - corresponds to structure (1) in figure 7

lattice parameter	x [Å]	y [Å]	z [Å]
a	7.95262233	0.00000000	0.00000000
b	0.00000000	7.95262233	0.00000000
c	-0.00017759	-0.00016645	12.01839646
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.74915328	0.75043956	0.27429288
Zr	0.24914507	0.25043396	0.27433639
Zr	0.24952589	0.75048856	0.77286097
Zr	0.24946261	0.25048944	0.77333317
Zr	0.74952622	0.75046127	0.77337966
Ti	0.74916852	0.25043450	0.26885508
Ti	0.24917994	0.75043199	0.26908201
Ti	0.74945440	0.25045491	0.76918852
S	0.24909443	0.75043875	-0.02598692
S	0.24909579	0.25043936	-0.02376574
S	0.74948203	0.25047194	0.45836718
S	0.24946584	0.75047782	0.45994090
S	0.74949946	0.75048515	0.47589682
S	0.24950598	0.25048066	0.47594498
S	0.74912627	0.25044097	0.95914239
S	0.74907805	0.75043737	0.97628761
Ba	0.49973476	1.00114575	0.08503928
Ba	0.49973574	0.49972738	0.08504311
Ba	0.50205262	0.49799622	0.58061191
Ba	0.50204947	1.00297585	0.58061235
Ba	0.99702618	0.49799413	0.58061462
Ba	0.99702961	0.00297781	0.58061572
Ba	0.99837843	0.00112845	1.08503346
Ba	0.99837634	0.49974473	1.08503474
O	0.74899341	0.00705728	0.22597570
O	0.74899541	0.49382129	0.22597712
O	-0.00760457	0.25043877	0.22598744
O	0.50560667	0.25043914	0.22601049
O	0.49305999	0.75044024	0.22682992
O	0.00494425	0.75044179	0.22684181
O	0.24899552	0.99450871	0.22685574
O	0.24899381	0.50636727	0.22686102
O	0.24959168	0.49983380	0.72028289
O	0.24959597	1.00115407	0.72028468
O	-0.00110908	0.75050489	0.72030361
O	0.50023913	0.75050087	0.72031330
O	0.50662592	0.25050122	0.72497705
O	-0.00744516	0.25049777	0.72500245
O	0.74958689	0.49347718	0.72501678
O	0.74958325	0.00752368	0.72501890

TABLE IX: -2.5% strained (in the ab plane) $BaZr_{0.625}Ti_{0.375}O_2S$ - corresponds to structure (2) in figure 7.

lattice parameter	x [Å]	y [Å]	z [Å]
a	7.93266313	0.00000000	0.00000000
b	0.00000000	7.93266313	0.00000000
c	-0.00000717	-0.08384452	12.07998412
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.24927498	0.75470523	0.27337553
Zr	0.24927893	0.25455949	0.27409270
Zr	0.24934453	0.24921785	0.77284352
Zr	0.74934124	0.24922028	0.77389347
Zr	0.24935142	0.74922196	0.77454876
Ti	0.74929491	0.23596038	0.27145771
Ti	0.74929179	0.73738514	0.27169693
Ti	0.74935364	0.74918594	0.76862579
S	0.24925823	0.25150016	-0.02500103
S	0.24926384	0.75146748	-0.02353997
S	0.74934868	0.74446985	0.46059236
S	0.74934681	0.24453651	0.46178512
S	0.24934015	0.74720087	0.47407328
S	0.24933807	0.24719316	0.47471654
S	0.74926084	0.75150166	0.95792738
S	0.74924287	0.25168336	0.97392097
Ba	0.50440701	1.00180574	0.08448079
Ba	0.50458252	0.50355335	0.08479065
Ba	0.50321005	0.49945865	0.58084541
Ba	0.99549036	0.49946021	0.58085161
Ba	0.50323227	0.99466651	0.58085805
Ba	0.99546835	-0.00533053	0.58086439
Ba	0.99408903	0.00180516	1.08446433
Ba	0.99391360	0.50355222	1.08477493
O	0.24921989	1.00496164	0.22129243
O	0.24922091	0.50486337	0.22156018
O	-0.00966819	0.75686881	0.22648923
O	0.50813754	0.75686996	0.22650447
O	-0.00991963	0.25647370	0.22748429
O	0.50838877	0.25647450	0.22749730
O	0.74923778	0.51388748	0.22777356
O	0.74923967	0.01162353	0.22861353
O	0.50056712	0.24851756	0.72029295
O	-0.00186566	0.24851812	0.72029898
O	0.24935199	0.49973398	0.72131510
O	0.24935162	0.99766455	0.72133866
O	0.74935247	-0.00831538	0.72422078
O	0.74935203	0.50521808	0.72423904
O	0.50670645	0.74858174	0.72521475
O	-0.00799689	0.74858223	0.72522554

TABLE X: 0% strained (in the ab plane) $BaZr_{0.625}Ti_{0.375}O_2S$ - corresponds to structure (3) in figure 7.

lattice parameter	x [Å]	y [Å]	z [Å]
a	8.14874960	0.00000000	0.00000000
b	0.00000000	8.14874960	0.00000000
c	0.31770661	-0.43904716	12.17360646
atom	x [f.c.]	y [f.c.]	z [f.c.]
Zr	0.78773640	0.76590142	0.28837179
Zr	0.75374861	0.74569300	0.76627496
Zr	0.25354634	0.24545586	0.76772701
Zr	0.75270719	0.24432067	0.76801671
Zr	0.25258590	0.74460783	0.76856618
Ti	0.73581813	0.21096655	0.28267945
Ti	0.30117757	0.26912139	0.28530756
Ti	0.23887558	0.70154981	0.28665055
S	0.24977205	0.25847050	-0.03313200
S	0.24134567	0.75202823	-0.03117444
S	0.76538749	0.22700501	0.47124051
S	0.26642136	0.23078700	0.47201359
S	0.26398931	0.72791253	0.47471915
S	0.76252659	0.72861087	0.48635790
S	0.75033295	0.76076006	0.96675582
S	0.74096345	0.24990526	0.96764343
Ba	0.49997120	0.51745085	0.08004598
Ba	0.48260559	1.00398994	0.08201497
Ba	1.01069763	0.48329789	0.58318187
Ba	1.01209357	-0.01360910	0.58348601
Ba	0.50875680	0.98594013	0.58354991
Ba	0.51019356	0.48407651	0.58399313
Ba	0.98430628	0.50081117	1.08015508
Ba	0.99991869	0.02067285	1.08201307
O	0.73266476	0.57905079	0.20224924
O	0.23483552	1.10180520	0.20705460
O	-0.09070773	0.27032895	0.20943015
O	0.41406524	0.77061399	0.21727674
O	0.72984501	-0.01040199	0.23012326
O	0.52260704	0.27266912	0.23593136
O	0.23563399	0.47978415	0.23622189
O	0.02748092	0.76907098	0.23921435
O	0.75512923	-0.00659355	0.71925730
O	0.50491806	0.24236155	0.71962985
O	0.00586544	0.74262629	0.71991933
O	0.25486558	0.49248693	0.72013655
O	0.00525988	0.24228251	0.72030376
O	0.25490679	0.99252628	0.72050365
O	0.75512263	0.49152935	0.72110306
O	0.50402970	0.74263773	0.72148672