Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Thermomechanical properties of zero thermal expansion materials from theory and experiments

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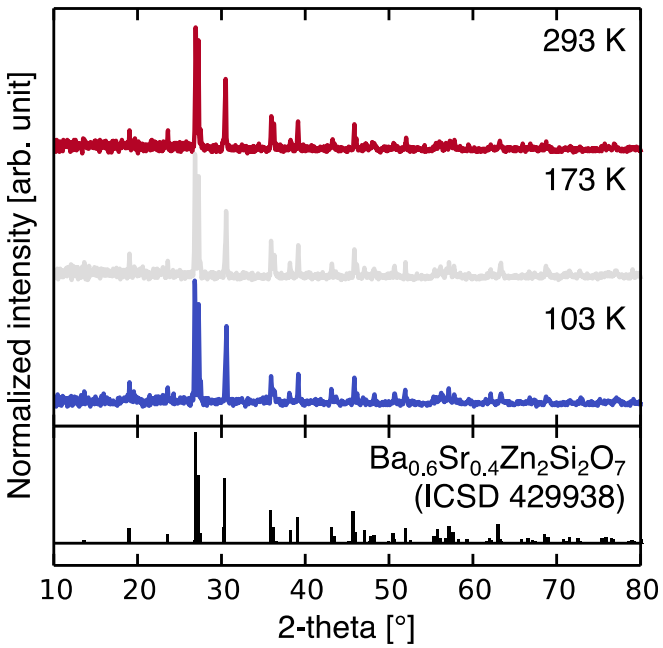

Figure S1 XRD-patterns of $Ba_{0.5}Sr_{0.5}Zn_2Si_2O_7$ at different temperatures.

Table S1 Cell parameters [Å] of $Ba_{1-x}Sr_xZn_2Si_2O_7$ solid solutions obtained by DFT simulations and experiments (exp).

x	cell parameter	DFT 0 K	exp 103 K	173 K	293 K
0.00	*a*	7.71	-	-	-
	b	12.95	-	-	-
	c	6.61	-	-	-
0.25	*a*	7.77	7.75	7.75	7.71
	b	12.94	12.96	12.97	12.98
	c	6.57	6.59	6.60	6.62
0.5	*a*	7.73	7.74	7.72	7.89
	b	12.93	12.95	12.94	12.95
	c	6.52	6.55	6.55	6.56
0.75	*a*	7.67	7.72	7.69	7.68
	b	12.93	12.93	12.93	12.93
	c	6.49	6.49	6.50	6.50

Table S2 Elements of the elastic stiffness C [GPa] and compliance S [TPa^{-1}] tensor calculated at the DFT level.

x	C_{aa}	C_{bb}	C_{cc}	C_{ab}	C_{ac}	C_{bc}	S_{aa}	S_{bb}	S_{cc}	S_{ab}	S_{ac}	S_{bc}
0.00	91	176	134	82	81	91	28	10	17	-6	-12	-3
0.25	88	177	137	81	81	91	30	10	17	-7	-13	-3
0.50	91	180	141	83	82	92	27	10	15	-7	-12	-3
0.75	83	183	145	81	81	92	33	10	15	-8	-13	-2

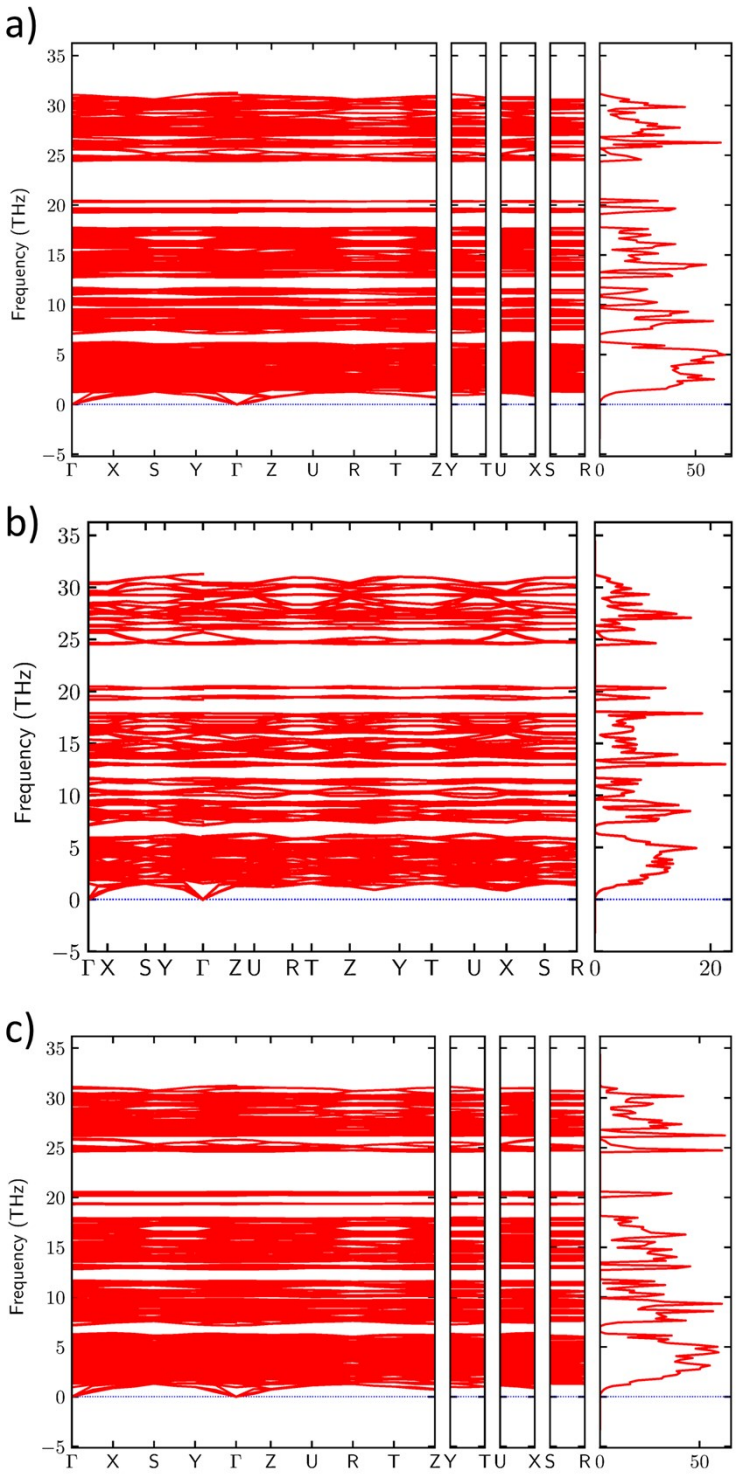

Figure S2 Phonon dispersion and density of states of $Ba_{1-x}Sr_xZn_2Si_2O_7$ solid solutions with a) x = 0.25, b) x=0.5 and c) 0.75.