Supplementary Information:
Theory-Guided Discovery of Pressure-Induced Transitions in Fast-Ion Conductor $BaSnF_4$

Authors

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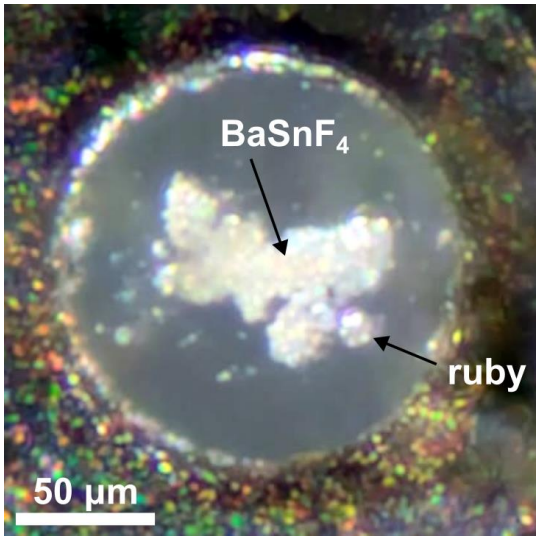
Supplementary Information



Supplementary Figure 1 – A typical loading of $BaSnF_4$ in a diamond anvil cell.

Supplementary Table 1 – Tetragonal *P*4*/nmm* $BaSnF_4$ lattice parameters from Rietveld XRD

Pressure (GPa)	*a* (Å)	*c* (Å)	Vol (Å^3)
0.00 outside DAC	*4.3538(4)*	*11.251(1)*	*213.27(5)*
0.00	4.3603(3)	11.418(1)	217.08(5)
0.08(5)	4.3581(3)	11.327(1)	215.13(5)
0.51(5)	4.3441(3)	11.116(2)	209.78(9)
1.08(5)	4.3292(3)	10.880(1)	203.90(5)
1.50(5)	4.3227(3)	10.755(1)	200.95(5)
1.56(5)	4.3248(4)	10.739(1)	200.86(5)
2.14(5)	4.3136(3)	10.606(1)	197.34(5)
2.52(5)	4.3098(3)	10.539(1)	195.76(5)
3.62(5)	4.2956(3)	10.362(1)	191.20(5)
4.35(5)	4.2873(4)	10.232(1)	188.08(5)
4.72(5)	4.2823(3)	10.202(1)	187.08(5)
5.89(5)	4.2702(3)	10.068(1)	183.58(5)
7.31(5)	4.2575(3)	9.920(1)	179.81(5)
8.48(5)	4.2495(3)	9.821(1)	177.34(5)

Supplementary Table 2 – Tetragonal *P*4*/nmm* $BaSnF_4$ lattice parameters from DFT

Pressure (GPa)	a (Å)	c (Å)	Vol (Å^3)
0	4.325	10.958	204.9762
0.8	4.311	10.764	200.0459
1.8	4.294	10.576	195.0049
3.1	4.276	10.393	190.0274
4.6	4.258	10.204	185.0043
6.3	4.241	10.007	179.9867
8.5	4.224	9.807	174.9782
11	4.206	9.609	169.9874
14.1	4.191	9.393	164.9832
17.7	4.181	9.154	160.0189
22.1	4.166	8.931	155.0025

Supplementary Table 3 – Monoclinic $P2_1/m$-I $BaSnF_4$ lattice parameters from XRD

Pressure (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	Vol (Å^3)
9.56(5)	4.247(1)	4.238(1)	9.783(5)	90.33(3)	176.1(2)
10.67(5)	4.246(1)	4.233(1)	9.759(5)	90.61(3)	175.4(2)
11.61(5)	4.247(1)	4.231(1)	9.744(7)	90.95(4)	175.1(2)
12.60(5)	4.250(2)	4.231(1)	9.72(1)	91.27(5)	174.8(3)

Supplementary Table 4 – Monoclinic $P2_1/m$-I $BaSnF_4$ lattice parameters from DFT

Pressure (GPa)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
6.2	4.252	4.252	9.955	89.972	90.002	89.992
8.3	4.238	4.238	9.744	89.993	89.999	89.986
10.8	4.225	4.225	9.524	89.998	89.998	89.993
13.9	4.211	4.211	9.306	89.992	89.998	89.996
17.5	4.197	4.198	9.081	89.994	89.999	89.992
21.9	4.182	4.185	8.856	89.995	89.998	89.996
27.2	4.166	4.196	8.581	90.002	90.000	89.911
32.3	4.141	4.197	8.344	90.055	90.000	89.990
39.2	4.105	4.190	8.139	90.159	90.000	89.984
47.6	4.064	4.167	7.972	90.291	89.999	89.992
57.7	4.019	4.139	7.815	90.443	90.000	89.985

Supplementary Table 5 – Monoclinic $P2_1/m$-II $BaSnF_4$ lattice parameters from DFT

Pressure (GPa)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
22.4	5.440	4.174	6.673	90.000	98.094	90.000
27.7	5.351	4.128	6.630	90.000	98.055	90.000
34.3	5.258	4.085	6.585	90.000	98.149	90.000
42.4	5.172	4.035	6.535	90.000	98.205	90.000
52.5	5.089	3.983	6.480	90.000	98.284	90.000
64.9	5.008	3.929	6.421	90.000	98.377	90.000
80.5	4.928	3.872	6.359	90.000	98.487	90.000

Supplementary Table 6 – Tetragonal *P*4*/nmm* $BaSnF_4$ atomic positions from XRD at 0.0 GPa.

Atom	Wyckoff position	Site symmetry	x	y	z	Occupancy
Ba1	2c	4mm	0.2500	0.2500	0.8709	1.0
Sn2	2c	4mm	0.2500	0.2500	0.3670	1.0
F1	4f	2mm	0.7500	0.2500	0.6948	1.0
F2	2a	-4m2	0.7500	0.2500	0.0000	1.0
F3	2c	4mm	0.2500	0.2500	0.1830	1.0

Supplementary Table 7 – Tetragonal *P*4*/nmm* $BaSnF_4$ atomic positions from DFT at 0.0 GPa.

Atom	Wyckoff position	Site symmetry	x	y	z	Occupancy
Ba1	2c	4mm	0.2500	0.2500	0.8640	1.0
Sn2	2c	4mm	0.2500	0.2500	0.3789	1.0
F1	4f	2mm	0.7500	0.2500	0.6805	1.0
F2	2a	-4m2	0.7500	0.2500	0.0000	1.0
F3	2c	4mm	0.2500	0.2500	0.1875	1.0

Supplementary Table 8 – Monoclinic $P2_1/m$-I $BaSnF_4$ atomic positions from XRD at 12.6 GPa.

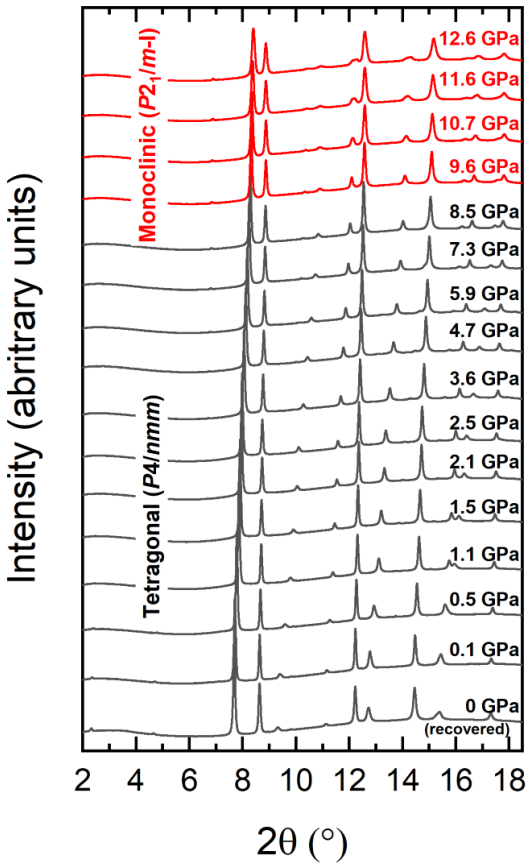
Atom	Wyckoff position	Site symmetry	x	y	z	Occupancy
Ba1	2e	m	0.7880	0.7500	0.1330	1.0
Sn2	2e	m	0.7760	0.7500	0.5870	1.0
F1	2e	m	0.2444	0.7500	0.6800	1.0
F2	2e	m	0.2496	0.7500	0.0200	1.0
F3	2e	m	0.7452	0.7500	0.8250	1.0
F4	2e	m	0.2536	0.7500	0.3000	1.0

Supplementary Table 9 – Monoclinic $P2_1/m$-I $BaSnF_4$ atomic positions from DFT at 11.0 GPa.

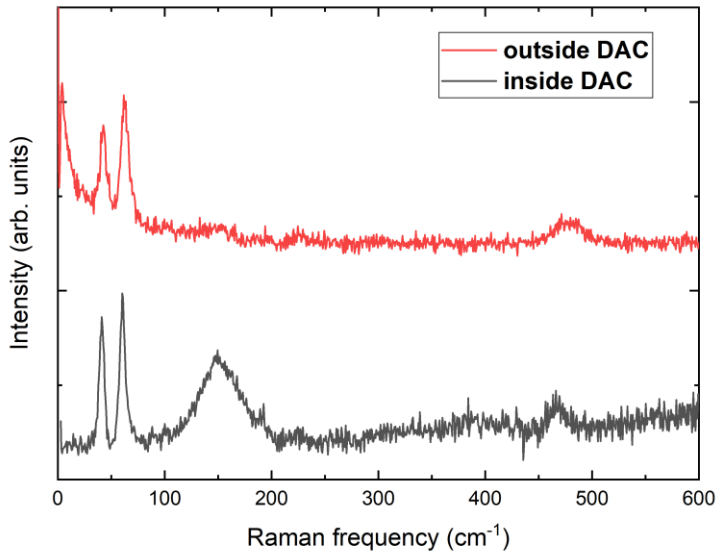
Atom	Wyckoff position	Site symmetry	x	y	z	Occupancy
Ba1	2e	m	0.7512	0.7500	0.1460	1.0
Sn2	2e	m	0.7500	0.7500	0.5923	1.0
F1	2e	m	0.2500	0.7500	0.6636	1.0
F2	2e	m	0.2500	0.7491	0.9999	1.0
F3	2e	m	0.7500	0.7521	0.8098	1.0
F4	2e	m	0.2500	0.7484	0.3364	1.0

Supplementary Table 10 – Monoclinic $P2_1/m$-II $BaSnF_4$ atomic positions from DFT at 34.0 GPa.

Atom	Wyckoff position	Site symmetry	x	y	z	Occupancy
Ba1	2e	m	0.7367	0.2500	0.9119	1.0
Sn2	2e	m	0.7163	0.7500	0.4607	1.0
F1	2e	m	0.5334	0.2500	0.2357	1.0
F2	2e	m	0.1232	0.7500	0.4507	1.0
F3	2e	m	0.9403	0.7500	0.7643	1.0
F4	2e	m	0.7792	0.7500	0.1336	1.0



Supplementary Figure 2 – Waterfall plot of all powder XRD data. Rietveld refinement was performed for each diffraction pattern shown. The corresponding lattice parameters are provided in Supplementary Tables 1 and 3. At 9.6 GPa the tetragonal symmetry undergoes a slight distortion to monoclinic symmetry wherein the β angle deviates from 90°.



Supplementary Figure 3 – Raman spectra of $BaSnF_4$ inside (black) and outside (red) of a diamond anvil cell (DAC).