Supplementary Information (SI) for Materials Advances.

Supporting Information

Elastic properties of Diverse Na-ion conductive Materials: A First-Principles Study

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Table S1. Elastic properties of hot-pressed pellets of $x$$Na_2S$ · $(100-x)P_2S_5$ (mol%) glass electrolytes prepared by a mechanochemical technique.[S1]

Formula	B / GPa	G / GPa	E / GPa	ν	B/G	MAV / $cm^3\ mol^{-1}$	Pellet density / $g\ cm^{-3}$	Relative density / %
$50Na_2S \cdot 50P_2S_5$	14.7	5.5	14.7	0.33	2.67	14.51	2.05	99.2
$67Na_2S \cdot 33P_2S_5$	20.2	7.0	18.7	0.35	2.91	14.33	2.01	99.0
$75Na_2S \cdot 25P_2S_5$	20.4	7.1	19.2	0.34	2.86	14.26	1.98	98.9

Table S2. Results of Bader charge analysis of various model crystal structures for $Na_{3-x}Sb_{1-x}W_xS_4$.

Element	Na_3SbS_4	$Na_{2.9375}Sb_{0.9375}W_{0.0625}S_4$	$Na_{2.875}Sb_{0.875}W_{0.125}S_4$
Na	+0.84, +0.85	+0.84, +0.85	+0.84, +0.85
Sb	+1.45	+1.44 ~ +1.46	+1.44 ~ +1.46
W	nonexistent	+1.63	+1.63
S	-1.00	-0.99, -1.00	-0.98 ~ -1.00

Table S3. Calculated elastic moduli of various Na_xY-type crystal and Na_3PO_4 crystal structures.

Formula	Crystal system	B / GPa	G / GPa	E / GPa	ν	B/G	MAV / $cm^3\ mol^{-1}$	Universal anisotropy
Na_2O	Cubic	55.21	36.03	88.78	0.23	1.53	8.28	0.19
Na_2S	Cubic	32.84	19.58	49.00	0.25	1.68	13.40	0
Na_2Se	Cubic	27.7	16.25	40.77	0.26	1.71	15.17	0.01
NaF	Cubic	56.99	37.08	91.42	0.23	1.54	7.40	0.31
NaCl	Cubic	24.08	14.63	36.50	0.25	1.65	13.84	0.24
NaBr	Cubic	23.93	13.94	35.02	0.26	1.72	15.41	0.74
NaI	Cubic	18.4	10.72	26.93	0.26	1.72	19.30	0.9
Na_3PO_4	Tetragonal	59.57	30.04	77.14	0.28	1.98	7.37	0.14

Table S4. Elastic moduli data obtained from the Materials Project. [S2]

Database	Type	Formula	Crystal system	B / GPa	G / GPa	v	A^U
mp-28782	Sulfide	α-Na_3PS_4	Tetragonal	23	11	0.29	0.41
mp-985584	Sulfide	β-Na_3PS_4	Cubic	23	6	0.37	4.71
mp-10167	Sulfide	Na_3SbS_4	Cubic	21	4	0.40	7.60
mp-8703	Selenide	Na_3SbSe_4	Cubic	19	6	0.37	0.82
mp-985586	Anti-perovskite	Na_3OBr	Cubic	32	22	0.22	0.02
mp-28602	Anti-perovskite	Na_3OCl	Cubic	33	22	0.22	0.16
mp-6150	NASICON	$Na_4Zr_2(SiO_4)_3$	Trigonal	91	48	0.28	1.15
mp-3405	Na-β-alumina	$NaAl_{11}O_{17}$	Hexagonal	152	70	0.30	1.27

Table S5. Detailed information on the solid electrolyte materials used in this study: the database from which the structural data were obtained, the number of k-points, and the lattice constants after structural optimization (used for the elastic tensor calculations). Crystal systems were determined based on the information provided in the corresponding database. It should be noted that the crystal system predicted from the lattice constants obtained after structural optimization differs from the one described.

Type	Formula	Crystal system	Database	k-points	a [Å]	b [Å]	c [Å]	a [°]	b [°]	g [°]
Sulfide	α-Na_3PS_4	Tetragonal	mp-28782	4×4×4	6.83	6.83	6.96	90.0	90.0	90.0
Sulfide	β-Na_3PS_4	Cubic	mp-985584	4×4×4	6.86	6.86	6.86	90.0	90.0	90.0
Sulfide	$NaPS_3$	Monoclinic	mp-1189520	4×3×2	6.55	7.56	8.92	90.0	89.4	90.0
Sulfide	Na_3SbS_4	Cubic	mp-10167	4×4×4	7.02	7.02	7.16	90.0	90.0	90.0
Sulfide	Na_3BS_3	Monoclinic	mp-29976	2×4×3	11.52	6.50	8.19	90.0	117.1	90.0
Sulfide	Na_5AlS_4	Orthorhombic	ICSD #31812	3×5×2	11.86	6.95	21.31	90.0	90.0	90.0
Sulfide	Na_3InS_3	Monoclinic	mp-29375	4×4×4	15.64	13.41	14.61	90.0	117.3	90.0
Sulfide	Na_4SnS_4	Tetragonal	mp-29628	4×4×5	7.71	7.71	6.91	90.0	90.0	90.0
Sulfide	Na_3AsS_4	Tetragonal	mp-138560	5×5×5	6.92	6.92	7.00	90.0	90.0	90.0
Selenide	Na_3PSe_4	Cubic	mp-1078419	4×2×2	7.18	7.19	7.19	90.0	90.0	90.0
Selenide	Na_3SbSe_4	Cubic	mp-8703	4×2×2	7.35	7.37	7.37	90.0	90.0	90.0
Anti-perovskite	Na_3OBr	Cubic	mp-985586	4×2×2	9.04	9.04	9.04	90.0	90.0	90.0
Anti-perovskite	Na_3OCl	Cubic	mp-28602	4×2×2	8.91	8.91	8.91	90.0	90.0	90.0
Anti-perovskite	$Na_3OBr_{0.5}Cl_{0.5}$	Cubic	Substitution in Na_3OCl	4×2×2	8.98	8.98	8.97	90.0	90.0	90.0

NASICON	$NaZr_2(PO_4)_3$	Trigonal	mp-6475	3×3×1	8.91	8.91	22.84	90.0	90.0	120.0
NASICON	$NaTi_2(PO_4)_3$	Trigonal	mp-6761	3×3×1	8.59	8.59	21.87	90.0	90.0	120.0
NASICON	$Na_3Sc_2(PO_4)_3$	Trigonal	mp-555608	4×4×2	9.12	9.12	21.81	90.0	90.0	90.0
NASICON	$Na_3Sc_2(PO_4)_3$	Monoclinic	mp-16956	3×4×4	15.45	8.97	9.10	90.0	123.5	90.0
NASICON	$Na_4Zr_2(SiO_4)_3$	Trigonal	mp-6150	3×3×1	9.29	9.29	22.07	90.0	90.0	120.0
NASICON	$Na_3Zr_2Si_2PO_{12}$	Triclinic	mp-532695	4×4×2	9.13	9.21	15.96	72.4	73.8	61.4
NASICON	$Na_3Zr_2Si_2PO_{12}$	Monoclinic	mp-2713548	3×4×4	15.88	9.16	9.09	90.0	90.0	90.0
NASICON	$Na_3Hf_2Si_2PO_{12}$	Monoclinic	mp-2713249	3×4×4	15.73	9.08	9.02	90.0	124.8	90.0
Na-β-alumina	$NaAl_{11}O_{17}$	Hexagonal	mp-3405	4×4×1	5.62	5.62	22.63	90.0	90.0	120.0
Other oxide	$NaAlO_2$	Orthorhombic	mp-9212	4×4×4	5.22	5.40	7.02	90.0	90.0	90.0
Other oxide	Na_5AlO_4	Orthorhombic	mp-13998	4×2×1	5.84	10.06	17.79	90.0	90.0	90.0
Other oxide	$Na_7Al_3O_8$	Triclinic	mp-556168	4×3×2	5.84	7.94	11.26	69.4	77.2	71.0
Other oxide	$Na_{14}Al_4O_{13}$	Monoclinic	mp-31008	4×1×4	5.93	27.07	5.93	90.0	119.6	90.0
Other oxide	$Na_{17}Al_5O_{16}$	Monoclinic	mp-559916	5×1×5	5.94	32.87	5.95	90.0	90.0	90.0
Other oxide	Na_3BO_3	Monoclinic	mp-30975	4×3×2	5.66	7.43	9.54	90.0	123.7	90.0
Other oxide	Na_4SiO_4	Triclinic	mp-7500	2×2×2	11.11	11.12	8.40	71.7	80.8	67.5
Other oxide	Na_3SbO_4	Monoclinic	mp-7404	6×6×6	5.45	6.58	5.77	90.0	109.5	90.0
Other oxide	Na_3NbO_4	Monoclinic	mp-27247	2×2×4	11.12	12.97	5.72	90.0	109.5	90.0
Chloride	$NaAlCl_4$	Orthorhombic	mp-23363	4×2×2	6.13	9.68	10.13	90.0	90.0	90.0
Chloride	$NaTaCl_6$	Monoclinic	mp-28179	4×2×2	12.75	13.64	18.84	90.0	91.1	90.0
Chloride	Na_2ZrCl_6	Trigonal	ICSD #143651	3×3×6	11.48	11.60	6.00	89.7	90.0	119.7
Chloride	Na_3ErCl_6	Monoclinic	mp-28542	6×5×3	6.71	7.21	11.95	90.0	123.1	90.0
Sulfide	$Na_{2.9375}Sb_{0.9375}W_{0.0625}S_4$	Cubic	Substitution in Na_3SbS_4	2×2×2	14.05	14.05	14.26	90.0	90.0	89.9
Sulfide	$Na_{2.875}Sb_{0.875}W_{0.125}S_4$	Cubic	Substitution in Na_3SbS_4	2×2×2	14.05	14.05	14.22	90.0	90.0	89.7
Hydride	$NaBH_4$	Cubic	mp-1190586	6×6×6	5.96	5.96	5.96	90.0	90.0	90.0
Hydride	$NaBH_4$	Tetragonal	mp-38725	8×8×6	4.22	4.22	5.74	90.0	90.0	90.0
Hydride	$NaBH_4$	Orthorhombic	mp-1190869	8×6×4	4.26	5.93	8.12	90.0	90.0	90.0
Hydride	NaB_3H_8	Orthorhombic	mp-1190348	7×6×4	4.38	5.70	7.60	90.0	90.0	90.0
Hydride	NaB_6H_6	Monoclinic	mp-978278	6×3×5	6.86	10.37	9.17	90.0	132.4	90.0
Hydride	$NaB_9H_{10}C$	Orthorhombic	mp-2646917	4×3×3	7.67	9.69	10.36	90.0	90.0	90.0
Hydride	$NaB_{11}H_{12}C$	Orthorhombic	mp-2646947	3×3×3	9.29	9.41	9.90	90.0	90.0	90.0

References

[S1] M. Nose, A. Kato, A. Sakuda, A. Hayashi and M. Tatsumisago, *J. Mater. Chem. A*, 2015, **3**, 22061.

[S2] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder and K. A. Persson, *APL Mater.*, 2013, **1**, 011002.