

Supplemental Materials

First-Principles Investigation of Auxetic Piezoelectric Effect in Nitride Perovskites

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TABLE SI. The plane-wave cut-off energy and the k -point meshes.

	ENCUT (eV)	k -point
ScMoN ₃	500	5 5 4
ScWN ₃	500	5 4 4
YMoN ₃	500	5 6 6
YWN ₃	500	5 6 6
LaMoN ₃	600	6 6 2
LaWN ₃	600	6 6 2

TABLE SII. Calculated elastic constants C_{ij} (GPa) of nitride perovskites ABN₃ (A = Sc, Y, La; B = Mo, W).

Compounds	C_{11}	C_{12}	C_{13}	C_{14}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
ScMoN ₃	293	114	191	-	335	146	286	95	137	35
ScWN ₃	468	150	142	-	423	142	331	72	116	155
YMoN ₃	402	136	128	-	250	108	261	49	108	133
YWN ₃	462	146	151	-	318	132	313	63	127	149
LaMoN ₃	303	167	94	37	303	94	246	52	52	68
LaWN ₃	353	197	116	43	353	116	307	68	68	78

TABLE SIII. Calculated elastic compliance constants S_{ij} (10^{-3} /GPa) of nitride perovskites ABN₃ (A = Sc, Y, La; B = Mo, W).

Compounds	S_{11}	S_{12}	S_{13}	S_{14}	S_{22}	S_{23}	S_{33}	S_{44}	S_{55}	S_{66}
ScMoN ₃	6.1	-0.4	-0.4	-	0.4	-1.7	6.9	10.5	7.3	28.1
ScWN ₃	2.6	-0.6	-0.8	-	2.9	-0.9	3.8	13.8	8.6	6.5
YMoN ₃	3.3	-1.3	-1.1	-	5.3	-1.6	5.0	20.6	9.2	7.5
YWN ₃	2.7	-0.8	-0.9	-	4.1	-1.3	4.2	15.8	7.9	6.7
LaMoN ₃	7.3	-4.7	-0.9	-8.6	7.3	-0.9	4.8	31.6	31.6	24.0
LaWN ₃	6.0	-3.9	-0.8	-6.3	6.0	-0.8	3.8	22.8	22.8	19.8

The Born elastic stability criteria¹ for ScMoN₃, ScWN₃, YMoN₃ and YWN₃:

$$C_{11} > 0, C_{22} > 0, C_{33} > 0, C_{44} > 0, C_{55} > 0, C_{66} > 0, C_{11} * C_{22} > C_{12}^2, \\ C_{11} * C_{22} * C_{33} + 2C_{12} * C_{13} * C_{23} - C_{11} * C_{23}^2 - C_{22} * C_{13}^2 - C_{33} * C_{12}^2 > 0$$

The Born elastic stability criteria¹ for LaMoN₃ and LaWN₃:

$$C_{11} > 0, C_{22} > 0, C_{33} > 0, C_{44} > 0, C_{55} > 0, C_{66} > 0, C_{11} - C_{12} > 0, \\ C_{13}^2 < 0.5 * C_{33} (C_{11} + C_{12}), C_{14}^2 < 0.5 * C_{44} * (C_{11} - C_{12})$$

References

1. F. Mouhat and F.-X. Coudert, *Phys. Rev. B*, 2014, **90**, 224104.