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Supporting Information:

Enhanced polarization in epitaxially strained monoclinic potassium niobate for lead-free electromechanical applications

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I. ELASTIC STABILITY

To determine the elastic stability for each KNbO_3 (KNO) polymorph, we have performed density-functional theory (DFT) calculations (with the PBEsol *xc* functional) to obtain their elastic stiffness constants, C_{ij} (as tabulated in Table S3) using the finite difference approach as implemented in the VASP code.

According to the proposed necessary and sufficient elastic stability conditions for each crystal systems [1], using our calculated C_{ij} values, we find that they all satisfy the Born stability criteria and note that the newly discovered monoclinic phase is metastable for KNO nano-materials.

For rhombohedral symmetry crystals, the elastic stability criteria is defined as follow [1],

$$C_{11} > |C_{12}|, \ C_{44} > 0, \ C_{13}^2 < \frac{1}{2}C_{33}(C_{11} + C_{12}), \ C_{14}^2 < \frac{1}{2}C_{44}(C_{11} - C_{12}) \equiv C_{44}C_{66}$$
 (1)

For orthorhombic symmetry crystals, the elastic stability criteria is defined as follow [1],

$$C_{11} > 0, C_{44} > 0, C_{55} > 0, C_{66} > 0, C_{11}C_{22} > C_{12}^2$$
, (2)

$$C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 > 0 \quad . \tag{3}$$

For tetragonal symmetry crystals, the elastic stability criteria is defined as follow [1],

$$C_{11} > |C_{12}|, C_{44} > 0, C_{66} > 0, 2C_{13}^2 < C_{33}(C_{11} + C_{12})$$
 (4)

For monoclinic symmetry crystals, the elastic stability criteria is defined as follow [2],

$$C_{11} > 0, C_{22} > 0, C_{33} > 0, C_{44} > 0, C_{55} > 0, C_{66} > 0$$
 , (5)

$$C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0 \quad , \tag{6}$$

$$C_{33}C_{55} - C_{35}^2 > 0, \ C_{44}C_{66} - C_{46}^2 > 0, \ C_{22} + C_{33} - 2C_{23} > 0 \quad , \tag{7}$$

$$\left[C_{22}(C_{33}C_{55} - C_{35}^2 + 2C_{23}C_{25}C_{35} - C_{23}^2C_{55} - C_{25}^2C_{33}\right] > 0 \quad , \tag{8}$$

$$2[C_{15}C_{25}(C_{33}C_{12} - C_{13}C_{23}) + C_{15}C_{35}(C_{22}C_{13} - C_{12}C_{23}) + C_{25}C_{35}(C_{11}C_{33} - C_{12}C_{13})] - [C_{15}^2(C_{22}C_{33} - C_{23}^2) + C_{25}^2(C_{11}C_{33} - C_{13}^2) + C_{35}^2(C_{11}C_{22} - C_{12}^2)] + gC_{55} > 0 (g = C_{11}C_{22}C_{33} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 + 2C_{12}C_{13}C_{23}) \quad .$$
(9)

II. RADIAL DISTRIBUTION FUNCTION

Based on ring statistics [3], the radial distribution function (RDF), g(r), is measured via the following equation:

$$g(r) = \frac{dn}{4\pi r^2 dr\rho}; \quad \rho = \frac{N}{V} \quad , \tag{10}$$

where dn is taken as the number of atoms at a distance between r and r + dr, and N and V are the number of atoms and the volume of the periodic simulation cell.

A deeper insight into the local structural distortion behavior under strain can be explained by the radial distribution function (RDF) plots (cf., Equation 10) in Figure S1. As seen in Figure S1c, we find that the longest peak split into two peaks when compressive/tensile strain is applied. This indicates that the cation displacement in the monoclinic structure undergoes a different local cation displacement direction when compressive/tensile strain is applied. We note that upon analyzing our simulated RDF data of the other phases in Figure S1, there are no peak split under strain.

III. BOND ELONGATION FROM QUADRATIC ELONGATION

The quadratic elongation, $\langle \lambda \rangle$ is a physical index to measure the degree of the off-center displacement of a central atom in octahedron unit [4], and conventionally used to study the individual contributions of the inter-octahedral distortions to the electronic band gap energy and optical property of the perovskite structure [5, 6].

The quadratic elongation, $\langle \lambda \rangle$ is given by following the equation:

$$\langle \lambda \rangle = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{l_i}{l_0} \right)^2 \tag{11}$$

where n is the coordination number of the central M atom (i.e., n = 6 refers to an octahedral environment); l_i is the distance from the central M atom to the ith coordinating atom; l_0 is the center-to-vertex distance of an ideal polyhedron of the same volume. If the difference between the measured and undistorted octahedron decreases, $\langle \lambda \rangle$ approaches the value of 1.

These quantities, however, provide only a rough measurement (simply estimate the lattice distortion isotropically) and cannot be taken as accurate index for axis-directional structural distortion, which is particularly important in ferroelectrics as polarizable atoms often drive certain local directional distortions from the structure, and understanding these directional distortion in terms of cartesian coordinate is important for unlocking the mechanisms that lead to spontaneous polarization and ferroelectricity. Furthermore, certain local directional distortions in octahedron result in profound alterations of the crystal structure, electronic structure, and polarization orientation [7].

We then have picture where the directional distortion in octahedron of a given perovskite provide a hint on the correlation between the structure, polarization orientation, and electronic structure, but a detailed anisotropic structural analysis or index is always necessary for estimating the electronic and polar properties.

Keeping this necessity in mind, we have defined the axis-decomposed directional quadratic elongation, $\langle \lambda_i \rangle$ of a given absolute x, y, and z cartesian coordinate system instead of a, b, and cunit cell vector based coordinate system to assess the directional off-centering distortion of central atom in octahedron. In this approach, we show how to derive the equation for coordinated $\langle \lambda_i \rangle$, which is useful to determine the distortion from three axis in a simple way. According to the Power Rule, Equation 11 can be derived in this way:

$$\langle \lambda \rangle = \frac{1}{6} \sum_{i=1}^{6} \left(\frac{l_i^2}{l_0^2} \right) \tag{12}$$

where the coordination number of the central M atom is 6 which, refer to an octahedral environment.

In order to understand the orientation-dependence of $\langle \lambda \rangle$, we express the bond length, l_i (centerto-vertex distance of the octahedron) as composition of a given absolute x, y, and z cartesian coordinate system of cartesian 3-space, where the vector of l_i is defined as

$$\vec{l}_i = \vec{M} - \vec{O} = \begin{pmatrix} x_1 - x_2 \\ y_1 - y_2 \\ z_1 - z_2 \end{pmatrix} = \begin{pmatrix} \Delta x_i \\ \Delta y_i \\ \Delta z_i \end{pmatrix}$$
(13)

where the vector of metal in octahedron, $\overrightarrow{M} = (x_1, y_1, z_1)$, the vector of vertex in octahedron, $\overrightarrow{O} = (x_2, y_2, z_2)$, and the vector of l_i , $\overrightarrow{l_i} = \overrightarrow{M} - \overrightarrow{O} = (\Delta x_i, \Delta y_i, \Delta z_i)$ are reformulated in this way. In this approach the bond length, l_i can be re-formulate as follow:

$$l_i = \sqrt{\overrightarrow{l_i}^2} = \sqrt{\Delta x_i^2 + \Delta y_i^2 + \Delta z_i^2} \tag{14}$$

where Δx_i^2 , Δy_i^2 , and Δz_i^2 are the difference of x, y, z vector components between center-to-vertex of the octahedron $\overrightarrow{l_i}$ to the second power.

Then we can re-write Equation 11, $\langle \lambda \rangle$ by substituting Equation 14 into Equation 12 as below:

$$\langle \lambda \rangle = \frac{1}{6} \left\{ \sum_{i=1}^{6} \left(\frac{\Delta x_i^2}{l_0^2} \right) + \sum_{i=1}^{6} \left(\frac{\Delta y_i^2}{l_0^2} \right) + \sum_{i=1}^{6} \left(\frac{\Delta z_i^2}{l_0^2} \right) \right\}$$
(15)

In short, $\langle \lambda \rangle$ could be defined as the following Equation:

$$\langle \lambda \rangle = \langle \lambda_x \rangle + \langle \lambda_y \rangle + \langle \lambda_z \rangle \tag{16}$$

where $\langle \lambda_x \rangle$, $\langle \lambda_y \rangle$, and $\langle \lambda_z \rangle$ are $\frac{1}{6} \sum_{i=1}^6 \left(\frac{\Delta x_i^2}{l_0^2}\right)$, $\frac{1}{6} \sum_{i=1}^6 \left(\frac{\Delta y_i^2}{l_0^2}\right)$, and $\frac{1}{6} \sum_{i=1}^6 \left(\frac{\Delta z_i^2}{l_0^2}\right)$ respectively.

Compared with conventional mean octahedral quadratic elongation parameters that only consider the isotropic distortion for octahedra, anisotropic quadratic elongation enable straightforward analysis for the degree of the directional off-center displacement of central atom in octahedron. However, we have found that the anisotropic quadratic elongation does not matched directly with the directional distortion under the biaxial strain due to the displacement values being squared (as seen in Equation 15). To be more specific, when compressive strain is applied in *tetra* KNO, the O anions along the y-direction moves the same distance according to strain in opposing directions, while the shift of Nb cation is along the z-direction. It means that the difference of $d_{\rm Nb-O}$ along the y-direction (between $d_{\rm Nb-O_y^-}$ and $d_{\rm Nb-O_y^+}$) is zero (i.e., no distortion in the y-direction). Here, if we square the difference in the center-to-vertex distances, then it will be misleading as the squared term contributes to making a spurious value despite no distortion in the y-direction.

One way to avoid this is by choosing the displacement value itself instead of absolute squared one, the bond elongation index $\overline{\lambda}_i$, thus providing directly the anisotropic distortion in octahedron. Here, we have found that the bond elongation index is a convenient and realistic measure of anisotropic distortion of central atom in octahedron. we re-define and propose the (revised) bond elongation index defined as following:

$$\left[\overline{\lambda}_x, \overline{\lambda}_y, \overline{\lambda}_z\right] = \frac{1}{n} \left[\sum_{i=1}^n \frac{\Delta x_i}{l_0}, \sum_{i=1}^n \frac{\Delta y_i}{l_0}, \sum_{i=1}^n \frac{\Delta z_i}{l_0} \right] \quad , \tag{17}$$

where Δx_i , Δy_i , and Δz_i are vector components of $\vec{l_i}$, which is a vector from *i* atom at polyhedron vertex to the center of the polyhedron, in the formal *x*, *y*, and *z* Cartesian axes. With the normalization of l_0 , this formulation allows us to investigate the anisotropic metal off-center displacement values in the polyhedron without taking a mean-field approach (as is in the case of $\langle \lambda \rangle$).

IV. FIGURES



Figure S1. Atomic and crystal structures of KNbO_3 polymorphs. (a) Rhombohedral 3m, (b) orthorhombic Amm2, (c) monoclinic Pm, (d) tetragonal P4mm, and (e) cubic $Pm\bar{3}m$. The corresponding space groups for each polymorph is shown and the K, Nb, and O atoms are depicted as white, blue, and red spheres, respectively.



Figure S2. Calculated radial distribution function (RDF), g(r), of KNbO₃ in (a) rhombohedral, (b) orthorhombic, (c) monoclinic, and (d) tetragonal phases within a coordination sphere of radius r. Yellow, blue, red lines indicate K–O, Nb–O, and O–O bonds.



Figure S3. Band structures and density-of-states (DOS) plots for (a) rhombohedral, (b) monoclinic, (c) orthorhombic, and (d) tetragonal phases of KNbO_3 . Yellow and blue lines in the band structures show the valence and conduction bands, respectively. Blue and red lines in the DOS indicate Nb 4d and O 2p states, while the grey show the total DOS.



Figure S4. Electron localization function (ELF) line profiles along the bonding path for (a) Si and (b) NaCl. The ELF spans from 0 to 1, where 1 denotes maximum localization of the electronic density.



Figure S5. Calculated directional bond elongation $(\bar{\lambda}_i)$, of KNbO₃ in (a) rhombohedral, (b) orthorhombic, (c) monoclinic, and (d) tetragonal phases with respect to strain from -4% to 4%. Here, the blue, red, black, and orange circles represent the *rhombo*, *ortho*, *mono*, and *tetra* KNbO₃ phases, respectively.



Figure S6. Spontaneous polarization P_s derived from K for the four polar polymorphs of KNbO₃ with respect to strain from -4% to 4%.



Figure S7. Calculated total energy differences, ΔE for the polar polymorphs of KNbO₃ as a function of biaxial strain, where the relative energy is referred to that of the cubic $(Pm\bar{3}m)$ phase at 0% strain.

V. TABLES

Table S1. Γ -centered **k**-point meshes and the corresponding number of irreducible **k**-points using the uniform reciprocal distance of **k** grid for structural optimization calculation. The last column gives the total calculated energy (*E*) per formula unit of KNbO₃.

	Space group	$\mathbf{k} ext{-spacing}$	k -grid	irreducible k -points	$E ({\rm eV/f.u.})$
$rhombo~{ m KNbO}_3$	R3m	0.20	$7 \times 7 \times 5$	32	-40.72965
		0.15	$9 \times 9 \times 7$	69	-40.72971
$or tho \ {\rm KNbO}_3$	Amm2	0.20	8 imes 6 imes 6	80	-40.72878
		0.15	$11 \times 8 \times 8$	150	-40.72878
$mono~{\rm KNbO}_3$	Pm	0.15	$11 \times 11 \times 11$	366	-40.72859
$tetra~{\rm KNbO}_3$	P4mm	0.20	$8 \times 8 \times 8$	75	-40.72328
		0.15	$11 \times 11 \times 11$	126	-40.72331

results are taken Refs. 10 and 11.	from Refs	s. 8 and 9	9. Other	relevant	exp	erimenta	al valu	es are also liste	ed and taken from
xc	Phase	a_0 (Å)	$b_0(\mathrm{\AA})$	$c_{0}\left(\mathrm{\AA}\right)$	α	β	γ	Space group	$\Delta H^{\rm f}({\rm eV/f.u.})$
PBEsol	rhombo	5.655	5.655	6.943	90	90	120	R3m	-13.248
	mono	4.027	3.962	4.017	90	90.17	90	Pm	-13.247
	or tho	3.962	5.680	5.696	90	90	90	Amm2	-13.247
	tetra	3.970	3.970	4.059	90	90	90	P4mm	-13.242
optB86b	rhombo	5.682	5.682	6.976	90	90	120	R3m	-13.964
	mono	4.050	3.980	4.029	90	90.17	90	Pm	-13.962
	or tho	3.979	5.707	5.723	90	90	90	Amm2	-13.963
	tetra	3.987	3.987	4.077	90	90	90	P4mm	-13.956
SCAN	rhombo	5.669	5.669	6.976	90	90	120	R3m	-14.306
	mono	4.044	3.960	4.041	90	90.22	90	Pm	-14.304
	or tho	3.960	5.702	5.731	90	90	90	Amm2	-14.304
	tetra	3.969	3.969	4.103	90	90	90	P4mm	-14.295
Theory a,b	rhombo	5.707	5.707	7.017	90	90	120	R3m	_
	mono	4.023	3.961	4.020	90	90.18	90	Pm	_
	or tho	3.980	5.744	5.771	90	90	90	Amm2	_
	tetra	3.992	3.992	4.128	90	90	90	P4mm	—
Experiment ^{c,d}	rhombo	5.651	5.651	6.947	90	90	120	R3m	_
	mono	4.050	3.992	4.021	90	90.1	90	Pm	—
	or tho	3.973	5.695	5.721	90	90	90	Amm2	—
	tetra	3.997	3.997	4.063	90	90	90	P4mm	_

Table S2. Optimized lattice parameters $(a_0, b_0, c_0 \text{ in Å}, \text{ and } \alpha, \beta, \text{ and } \gamma \text{ in }^\circ)$, crystallographic space group, and formation energies $(\Delta H^{\rm f} \text{ in eV/f.u.})$ of bulk KNbO₃ polymorphs, calculated using PBEsol, optB86b, and SCAN xc functionals with comparison of other theoretical and experimental literatures. All theory results are taken from Refs. 8 and 9. Other relevant experimental values are also listed and taken from Refs. 10 and 11.

 a Reference 8

 b Reference 9

 c Reference 10

 d Reference 11

Phase	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{14}	C_{15}	C_{23}	C_{25}	C_{35}	C_{46}	BHc
rhombo	245.9	-	245.6	37.9	-	73.6	98.6	75.3	-31.2	-	-	-	-	-	Satisfy
mono	173.2	374.6	177.4	92.4	88.0	91.9	91.2	109.7	-	5.1	95.0	-1.4	6.0	0.8	Satisfy
or tho	374.3	241.2	219.1	33.0	91.0	93.0	91.6	94.4	-	-	54.2	-	-	-	Satisfy
tetra	387.1	-	169.9	90.0	-	96.0	85.5	84.1	-	-	-	-	-	-	Satisfy

Table S3. Calculated elastic constants of polar KNbO_3 polymorphs with the PBEsol *xc* functional. The elastic stability of these polymorphs are determined by satisfying the Born-Huang criteria (BHc).

Phase	xc	E_g (eV)	$\epsilon_{\rm VBM} \rightarrow \epsilon_{\rm CBM}$
rhombo	HSE06@PBEsol	3.47	$T\to \Gamma$
	PBEsol	2.17	$T\to \Gamma$
	SCAN	2.76	$T\to \Gamma$
	optB86b	2.16	$T\to \Gamma$
mono	HSE06@PBEsol	3.26	$\mathbf{R} \to \Gamma$
	PBEsol	1.91	$\mathbf{R}\to \Gamma$
	SCAN	2.54	$\mathbf{R}\to \Gamma$
	optB86b	1.93	$\mathbf{R}\to \Gamma$
or tho	HSE06@PBEsol	3.26	$T\to \Gamma$
	PBEsol	1.96	$T\to \Gamma$
	SCAN	2.44	$T\to \Gamma$
	${ m optB86b}$	2.00	$T\to \Gamma$
tetra	HSE06@PBEsol	2.88	$\mathbf{A} \to \Gamma$
	PBEsol	1.55	$\mathbf{A} \to \Gamma$
	SCAN	1.84	$\mathbf{A} \to \Gamma$
	optB86b	1.58	$\mathbf{A} \to \Gamma$

Table S4. DFT-calculated band-gap energy (ϵ_{gap}) of KNbO₃ polymorphs using various *xc* functionals. All polymorphic phases exhibit an indirect band gap. The positions of valence band maximum (ϵ_{VBM}) and the conduction band minimum (ϵ_{CBM}) are determined from the electronic band structure diagrams.

Phase	Space group	ion	Wyckoff position	xx	yy	zz	xy	xz	yx	yz	zx	zy
tetra	P4mm	Κ	(1b)	1.14	1.14	1.19	-	-	-	-	-	-
		Nb	(1a)	9.18	9.18	7.15	-	-	-	-	-	-
		Ο	(2c)	-7.01	-1.75	-1.43	-	-	-	-	-	-
		Ο	(1a)	-1.56	-1.56	-5.48	-	-	-	-	-	-
or tho	Amm2	Κ	(2b)	1.14	1.18	1.16	-	-	-	-	-	-
		Nb	(2a)	8.99	8.13	7.30	-	-	-	-	-	-
		Ο	(4d)	-1.61	-3.91	-3.47	-	-	-	-2.30	-	-2.15
		Ο	(2b)	-6.91	-1.49	-1.53	-	-	-	-	-	-
mono	Pm	Κ	(1a)	1.17	1.15	1.16	-	0.01	-	-	0.01	-
		Nb	(1b)	7.59	9.01	7.89	-	0.41	-	-	0.41	-
		Ο	(1a)	-1.49	-6.92	-1.53	-	0.02	-	-	0.02	-
		Ο	(1b)	-1.45	-1.63	-6.05	-	-0.29	-	-	-0.14	-
		Ο	(1b)	-5.82	-1.60	-1.47	-	-0.15	-	-	-0.29	-
rhombo	R3m	Κ	(3a)	1.17	1.17	1.15	-	-	-	-	-	-
		Nb	(3a)	8.43	8.43	7.45	-	-	-	-	-	-
		0	(9b)	-1.51	-4.89	-2.87	-	-	-	2.20	-	2.05

Table S5. Born effective charges (Z^\ast) of unstrained ${\rm KNbO}_3$ polymorphs.

	Space group	xc functional	$\Delta E ({\rm meV/f.u.})$
$rhombo~{ m KNbO}_3$	R3m	HSE06@PBEsol	-56.76
$or tho~{\rm KNbO}_3$	Amm2	PBEsol HSE06@PBEsol PBEsol	-28.33 -56.32 -27.66
$mono~{\rm KNbO}_3$	Pm	HSE06@PBEsol PBEsol	-55.31 -27.48
$tetra~{\rm KNbO}_3$	P4mm	HSE06@PBEsol PBEsol	-45.20 -22.16

Table S6. The calculated energy difference (ΔE) with respect to the cubic $(Pm\bar{3}m)$ phase using HSE06 xc functional based on the optimized structure from PBEsol xc functional (HSE06@PBEsol) and the calculated ΔE with respect to the cubic $(Pm\bar{3}m)$ phase using PBEsol xc functional.

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