Supplementary Data

Data-Driven Screening of Stable Lead-Free Piezoelectric Materials using Machine Learning and Graph-Based Models

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Table S1. Best hyperparameter values found by Optuna for each model.

Model	Hyperparameter	Symbol	Value
XGBoost	Number of trees	T	700
	Learning rate	η	1.673×10^{-2}
	Maximum tree depth	d	8
	Row subsampling	ρ_{row}	0.858
	Column subsampling	ρ_{col}	0.950
	Minimum child weight	min_child_weight	13
	L1 regularisation	α	3.884×10^{-2}
	L2 regularisation	λ	4.714
LightGBM	Number of trees	T	300
	Learning rate	η	3.687×10^{-2}
	Number of leaves	num_leaves	66
	Min. samples per leaf	min_child_samples	5
	Row subsampling	ρ_{row}	0.505
	Column subsampling	ρ_{col}	0.662
	L1 regularisation	α	1.147
	L2 regularisation	λ	0.257
CatBoost	Number of iterations	T	1000
	Learning rate	η	3.658×10^{-2}
	Tree depth	d	8
	L2 leaf regularisation	λ	4.740×10^{-2}
	Row subsampling	ρ_{row}	0.863
	Column subsampling (level)	ρ_{col}	0.966
SVM	Regularisation	C	2.157
	Tube width	ε	7.975×10^{-2}
	Kernel width	γ	`auto`
DNN	Hidden dimension	h	512
	Number of residual blocks	N_{blocks}	4
	Dropout rate	p_{drop}	0.273
	Learning rate	η	3.125×10^{-4}
	Weight decay	λ_{wd}	6.848×10^{-4}
TabNet	Feature dimension	$N_d = N_a$	64
	Number of decision steps	N_{steps}	3
	Sparsity regularisation	γ_{TN}	1.023
	Learning rate	η	2.846×10^{-3}
	Batch normalisation momentum	m	0.297
CGCNN	Hidden dimension	h	64
	Number of conv. layers	N_{conv}	5
SchNet	Hidden dimension	h	64
	Number of interactions	N_{int}	4
MPNN	Hidden dimension	h	64
	Number of message steps	N_{steps}	3
MEGNet	Hidden dimension	h	32
	Number of blocks	N_{blocks}	5
GATGNN	Hidden dimension	h	128
	Number of attention heads	K	8
	Number of GAT layers	N_{layers}	7

Model	Hyperparameter	Symbol	Value
CrystalAttentionNet	Hidden dimension	h	64
	Number of attention heads	K	2
	Number of attention layers	N_{layers}	2
ALIGNN	Hidden dimension	h	32
	Number of ALIGNN layers	N_{layers}	2

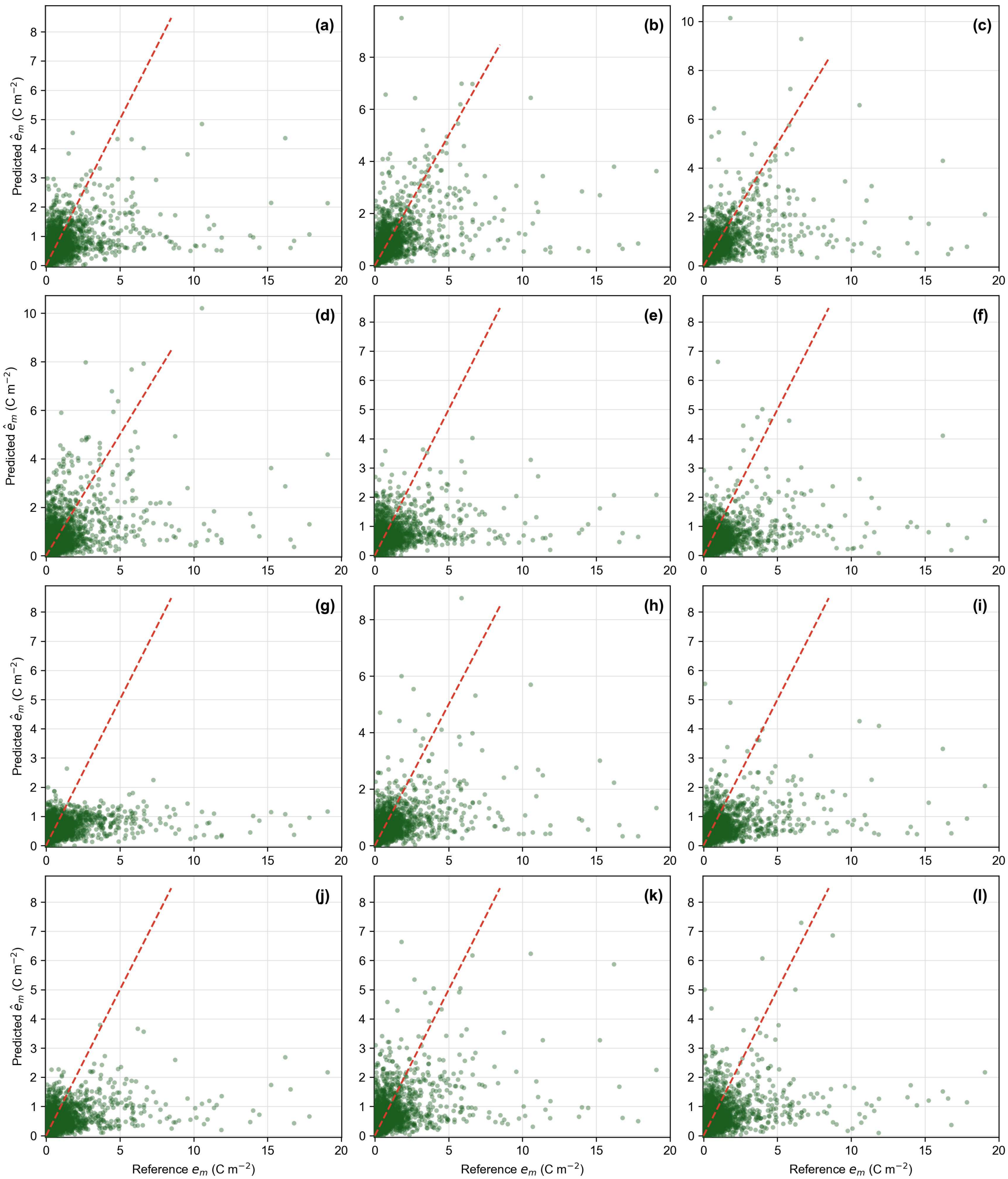

Fig. S1. Parity plots for the rest of evaluated models. Dashed line is the ideal 1:1 correspondence. (a) SVM; (b) LightGBM; (c) CatBoost; (d) DNN; (e) TabNet; (f) CGCNN; (g) SchNet; (h) MPNN; (i) MEGNet; (j) CATGNN; (k) CrystalAttn; (l) ALIGNN.

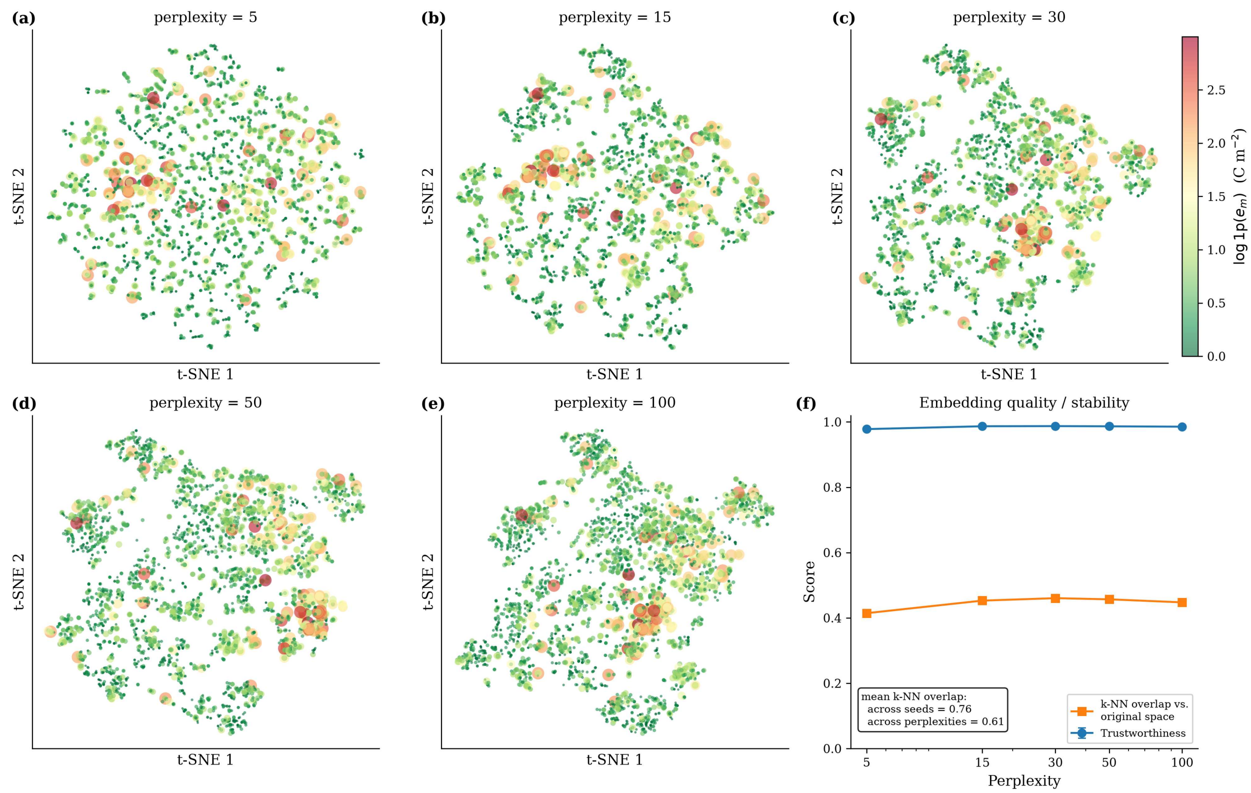

Fig. S2. Robustness of the t-SNE visualisation (Fig. 3 of the main text) to its hyperparameters. (a)–(e) t-SNE embeddings of the 3303 training materials computed at perplexities 5, 15, 30, 50 and 100 (random initialisation, fixed seed); point colour encodes $\log 1\mathrm{p}(e_m)$ and point area is proportional to e_m. Although the global arrangement of the map changes appreciably with perplexity, the grouping of the high-e_m (red) compounds into a few regions persists across all settings. (f) Embedding-quality diagnostics as a function of perplexity: the trustworthiness (fraction of local neighbourhoods preserved from the original feature space) stays high (0.98–0.99) for every perplexity, and the average 15-nearest-neighbour overlap with the original space is essentially flat. The inset reports the mean k-NN neighbourhood overlap between *independent* embeddings: 0.76 across random seeds and 0.61 across perplexities, quantifying the stochastic sensitivity that the embedding nonetheless retains. The t-SNE map is therefore used only as a qualitative exploratory aid.

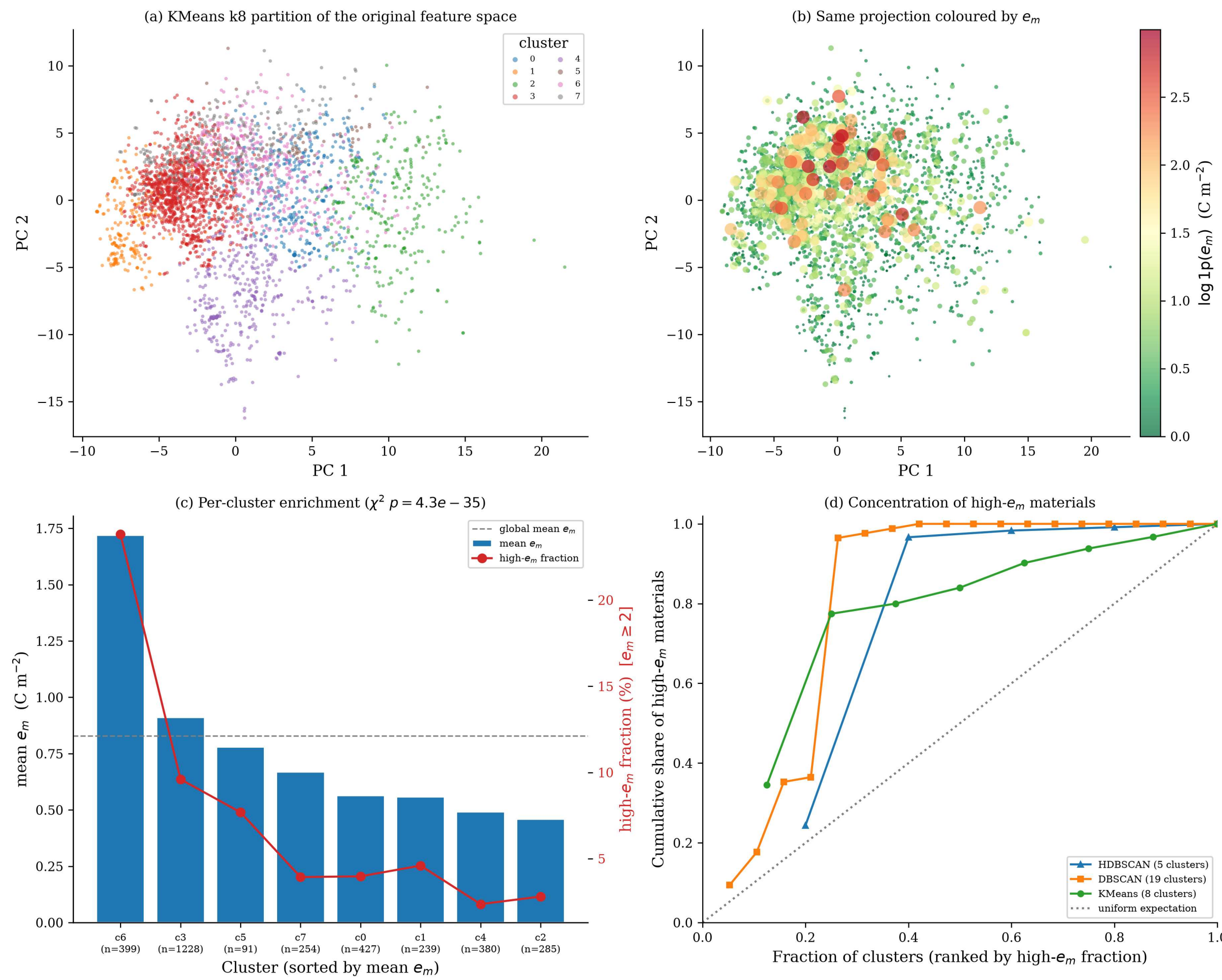

Fig. S3. Corroboration of the qualitative t-SNE clustering with robust, non-stochastic clustering applied to the original 50-principal-component feature space. (a) The KMeans ($k = 8$) partition shown on the first two principal components. (b) The same projection coloured by $\log 1\text{p}(e_m)$; the high-e_m compounds occupy a restricted region. (c) Per-cluster mean e_m (bars, left axis) and high-e_m fraction ($e_m \geq 2$ C/m^2; red line, right axis) for the KMeans reference partition; a χ^2 test of independence between cluster membership and the high/low-e_m label is highly significant ($p \approx 4 \times 10^{-35}$). A single oxide/transition-metal cluster, dominated by O, Ta, W and Bi, concentrates the high-e_m materials, in agreement with the SHAP feature attributions and the elemental-frequency analysis of the main text. (d) Cumulative share of all high-e_m materials captured by the top-k clusters (ranked by high-e_m fraction) for three independent clustering algorithms; every curve lies far above the uniform-expectation diagonal, confirming that high-e_m materials are concentrated in a small number of composition-based clusters. The same conclusion is reached with HDBSCAN ($p \approx 3.5 \times 10^{-22}$) and DBSCAN ($p \approx 2.7 \times 10^{-18}$), none of which involves a stochastic dimensionality-reduction step.

S2. DFT piezoelectric tensors and SVD-based piezoelectric moduli e_m of the validation set

This section reports the complete first-principles piezoelectric tensors computed for the twenty compounds of the DFT validation set (ten predicted-high and ten predicted-low materials; see Sections 2.7 and 3.5 of the main text). All tensors are piezoelectric stress tensors $e_{i\mu}$ in units of $\mathrm{C/m^2}$, given as 3×6 matrices with the row index $i = x, y, z$ (electric-polarisation direction) and the column index μ running over the six Voigt strain components.

Column ordering. The raw VASP output (`PIEZOELECTRIC TENSOR`) prints the columns in the order XX, YY, ZZ, XY, YZ, ZX. Here the columns have been *reordered* to the standard Voigt convention

$$\mu = 1, \ldots, 6 \;\longleftrightarrow\; xx,\ yy,\ zz,\ yz,\ zx,\ xy,$$

so that the matrices can be compared directly with the tensors reported by the Materials Project. (Note that a column permutation is an orthogonal transformation and therefore does *not* change the singular values used below.)

Contributions. For each material three matrices are given:

- $\mathbf{e}^{\mathrm{el}}$: electronic (clamped-ion) contribution, i.e. the `PIEZOELECTRIC TENSOR (including local field effects)` block;
- $\mathbf{e}^{\mathrm{ion}}$: ionic (internal-relaxation) contribution, i.e. the `PIEZOELECTRIC TENSOR IONIC CONTR` block;
- $\mathbf{e}^{\mathrm{tot}} = \mathbf{e}^{\mathrm{el}} + \mathbf{e}^{\mathrm{ion}}$: the total (relaxed-ion) piezoelectric tensor, which is the quantity that is compared with experiment and with the Materials Project entries.

Piezoelectric modulus e_m. Following the current Materials Project definition, the reported modulus is the largest singular value of the total piezoelectric matrix. Writing the singular value decomposition of the 3×6 total tensor as

$$\mathbf{e}^{\mathrm{tot}} = \mathbf{U}\,\mathbf{\Sigma}\,\mathbf{V}^{\top}, \qquad \mathbf{\Sigma} = \mathrm{diag}(\sigma_1, \sigma_2, \sigma_3), \quad \sigma_1 \geq \sigma_2 \geq \sigma_3 \geq 0,$$

the piezoelectric modulus is

$$e_m \;=\; \sigma_{\max}\big(\mathbf{e}^{\mathrm{tot}}\big) \;=\; \sigma_1 \;=\; \max_{\|\mathbf{s}\|=1} \big\|\mathbf{e}^{\mathrm{tot}}\,\mathbf{s}\big\|_2,$$

i.e. the spectral (ℓ_2-operator) norm of the tensor: the largest polarisation magnitude that can be produced by a unit-norm strain (in Voigt representation). Equivalently, $e_m = \sqrt{\lambda_{\max}(\mathbf{e}^{\mathrm{tot}}\,\mathbf{e}^{\mathrm{tot}\top})}$. All three singular values are listed for each material.

Caveat. A few entries ($Ba_3Ti_2O_7$, Rb_2ZrO_3, $RbCaCl_3$, $SrTa_2Bi_2O_9$, $SrTaNO_2$, YWN_3) show anomalously large ionic contributions (up to $\sim 10^2$ $\mathrm{C/m^2}$), which usually signals a structure close to a lattice instability or an insufficiently converged ionic relaxation. Their e_m values should be treated with caution (see the discussion in Section 3.5 of the main text).

Table S2. DFT piezoelectric modulus $e_m = \sigma_{\max}(\mathbf{e}^{\mathrm{tot}})$ of the twenty validation-set compounds, ranked by decreasing e_m. Entries marked with † belong to the anomalously-large-ionic-contribution group discussed in the text. MP-ID and SG (space-group number) identify the specific Materials Project polymorph used for each formula.

#	Material	MP-ID	SG #	e_m (C/m^2)
1	$SrTaNO_2$†	mp-756088	7	103.00429
2	Rb_2ZrO_3†	mp-752401	9	17.63571
3	$Ba_3Ti_2O_7$†	mp-770118	42	13.38400
4	YWN_3†	mp-989576	161	9.27954
5	$RbCaCl_3$†	mp-2795318	99	4.90767
6	$SrTa_2Bi_2O_9$†	mp-23089	36	2.92973
7	$TiPN_3$	mp-989613	38	1.90220
8	Bi_2O_3	mp-1105780	159	1.79365
9	$BaTiO_3$	mp-558125	20	0.90196
10	Cu_3BiS_3	mp-607291	19	0.72870
11	LiCuS	mp-2724538	31	0.69431
12	$Ca_3Sn_2O_7$	mp-1374018	36	0.47126
13	ZnP_4	mp-14587	92	0.42564
14	$Ba(LaSe_2)_2$	mp-37741	122	0.31460
15	$BaSiO_3$	mp-7339	19	0.29994
16	Al_2S_3	mp-2654	169	0.26651
17	Li_8SiO_6	mp-28549	185	0.19800
18	$CuBSe_2$	mp-983565	122	0.11530
19	$MgSnP_2$	mp-1009083	122	0.11255
20	$MoW_3(SeS_3)_2$	mp-1029037	156	0.05073

Piezoelectric tensors, material by material

Al_2S_3

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.01522 & 0.08602 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.08602 & 0.01522 & 0.00000 \\ 0.13570 & 0.13570 & -0.27408 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.00503 & -0.11704 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.11704 & 0.00503 & 0.00000 \\ -0.05675 & -0.05675 & 0.51608 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.02025 & -0.03102 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.03102 & 0.02025 & 0.00000 \\ 0.07895 & 0.07895 & 0.24200 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 0.26651, 0.03704, 0.03704

Piezoelectric modulus: $e_m = 0.26651$ C/m^2

$Ba(LaSe_2)_2$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.16671 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.16671 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.14165 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.14789 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.14789 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.10557 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.31460 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.31460 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.24722 \end{pmatrix}$$

Singular values: 0.31460, 0.31460, 0.24722

Piezoelectric modulus: $e_m = 0.31460$ C/m^2

$Ba_3Ti_2O_7$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.04197 \\ -0.02092 & -0.04496 & -0.08610 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.01815 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -11.61830 \\ -8.28334 & -10.44914 & -0.12530 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00698 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -11.57633 \\ -8.30426 & -10.49410 & -0.21140 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.01117 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 13.38400, 11.57633, 0.01117

Piezoelectric modulus: $e_m = 13.38400$ C/m^2

$BaSiO_3$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.00542 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.01398 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.01449 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.07314 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.02198 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.31443 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.06772 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00800 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.29994 \end{pmatrix}$$

Singular values: 0.29994, 0.06772, 0.00800

Piezoelectric modulus: $e_m = 0.29994$ C/m^2

$BaTiO_3$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.04257 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.04253 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.05192 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.37924 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.42342 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.85004 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.33667 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.38089 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.90196 \end{pmatrix}$$

Singular values: 0.90196, 0.38089, 0.33667

Piezoelectric modulus: $e_m = 0.90196$ C/m^2

$\mathbf{Bi_2O_3}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.01039 & -0.01039 & 0.00000 & 0.00000 & 0.24745 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.24745 & 0.00000 & -0.01039 \\ 0.42971 & 0.42971 & -0.90503 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} -0.30926 & 0.30926 & 0.00000 & 0.00000 & 0.93178 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.93178 & 0.00000 & 0.30926 \\ 0.83800 & 0.83800 & 0.95971 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} -0.29887 & 0.29887 & 0.00000 & 0.00000 & 1.17923 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 1.17923 & 0.00000 & 0.29887 \\ 1.26771 & 1.26771 & 0.05468 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 1.79365, 1.25269, 1.21651

Piezoelectric modulus: $e_m = 1.79365$ C/m^2

$\mathbf{Ca_3Sn_2O_7}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.02893 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.03630 & 0.00000 & 0.00000 \\ 0.02433 & 0.02801 & -0.03710 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.04508 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.09830 & 0.00000 & 0.00000 \\ -0.17991 & -0.23172 & 0.43255 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.07401 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.06200 & 0.00000 & 0.00000 \\ -0.15558 & -0.20371 & 0.39545 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 0.47126, 0.07401, 0.06200

Piezoelectric modulus: $e_m = 0.47126$ C/m^2

$\mathbf{Cu_3BiS_3}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.03543 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.04509 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.13311 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.07664 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.68361 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.03085 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.04121 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.72870 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.10226 \end{pmatrix}$$

Singular values: 0.72870, 0.10226, 0.04121

Piezoelectric modulus: $e_m = 0.72870$ C/m^2

$\mathbf{CuBSe_2}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.38006 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.38006 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.46737 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.43759 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.43759 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.35207 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.05753 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.05753 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.11530 \end{pmatrix}$$

Singular values: 0.11530, 0.05753, 0.05753

Piezoelectric modulus: $e_m = 0.11530$ C/m^2

$\mathbf{Li_8SiO_6}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.06223 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.06223 & 0.00000 & 0.00000 \\ 0.07556 & 0.07556 & -0.13943 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.00093 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.00093 & 0.00000 & 0.00000 \\ 0.04051 & 0.04051 & 0.25016 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.06130 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.06130 & 0.00000 & 0.00000 \\ 0.11607 & 0.11607 & 0.11073 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 0.19800, 0.06130, 0.06130

Piezoelectric modulus: $e_m = 0.19800$ C/m^2

LiCuS

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.22528 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.22529 & 0.00000 & 0.00000 \\ 0.22359 & -0.22305 & -0.00017 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.19652 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.16963 & 0.00000 & 0.00000 \\ 0.40537 & 0.04755 & 0.23613 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.42180 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.39492 & 0.00000 & 0.00000 \\ 0.62896 & -0.17550 & 0.23596 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 0.69431, 0.42180, 0.39492

Piezoelectric modulus: $e_m = 0.69431$ C/m^2

$\mathbf{MgSnP_2}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.59129 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.59129 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.62782 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.70384 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.70384 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.72629 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.11255 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.11255 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.09847 \end{pmatrix}$$

Singular values: 0.11255, 0.11255, 0.09847

Piezoelectric modulus: $e_m = 0.11255$ C/m^2

$\mathbf{MoW_3(SeS_3)_2}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00011 & 0.00310 \\ 0.00310 & -0.00310 & 0.00000 & 0.00011 & 0.00000 & 0.00000 \\ 0.00022 & 0.00022 & -0.00035 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00004 & 0.03277 \\ 0.03277 & -0.03277 & 0.00000 & 0.00004 & 0.00000 & 0.00000 \\ 0.00268 & 0.00268 & 0.00556 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00015 & 0.03587 \\ 0.03587 & -0.03587 & 0.00000 & 0.00015 & 0.00000 & 0.00000 \\ 0.00290 & 0.00290 & 0.00521 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 0.05073, 0.03587, 0.00663

Piezoelectric modulus: $e_m = 0.05073$ C/m^2

$\mathbf{Rb_2ZrO_3}$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 10.52071 & 3.32904 \\ 0.05536 & -0.44142 & -0.11750 & -0.20682 & 0.00000 & 0.00000 \\ 0.05702 & 0.61776 & -0.67172 & -0.28148 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 6.76770 & 0.15367 \\ -0.91582 & -0.12093 & 2.19670 & 1.98850 & 0.00000 & 0.00000 \\ -1.41882 & -5.11770 & -7.03905 & -3.45526 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 17.28841 & 3.48271 \\ -0.86046 & -0.56235 & 2.07920 & 1.78168 & 0.00000 & 0.00000 \\ -1.36180 & -4.49994 & -7.71077 & -3.73674 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 17.63571, 9.97436, 2.14228

Piezoelectric modulus: $e_m = 17.63571$ C/m^2

$RbCaCl_3$

$$\mathbf{e}^{\rm el} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.21394 & 0.21633 \\ 0.04532 & -0.02045 & 0.06683 & -0.10942 & 0.00000 & 0.00000 \\ -0.03091 & -0.16611 & 0.16063 & 0.07384 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\rm ion} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 5.11268 & -0.51222 \\ 0.42511 & -0.21137 & 0.09341 & 0.28414 & 0.00000 & 0.00000 \\ 0.19192 & 0.87862 & -0.14655 & 0.38729 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\rm tot} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 4.89874 & -0.29589 \\ 0.47043 & -0.23182 & 0.16024 & 0.17472 & 0.00000 & 0.00000 \\ 0.16101 & 0.71251 & 0.01408 & 0.46113 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 4.90767, 0.86402, 0.57545

Piezoelectric modulus: $e_m = 4.90767$ C/m^2

$SrTa_2Bi_2O_9$

$$\mathbf{e}^{\rm el} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.01225 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.08853 & 0.00000 & 0.00000 \\ -0.06315 & 0.02428 & 0.11328 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\rm ion} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & -2.94198 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.11454 & 0.00000 & 0.00000 \\ -0.48286 & -1.12929 & -2.10916 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\rm tot} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & -2.92973 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.20307 & 0.00000 & 0.00000 \\ -0.54601 & -1.10501 & -1.99588 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 2.92973, 2.34579, 0.20307

Piezoelectric modulus: $e_m = 2.92973$ C/m^2

$SrTaNO_2$

$$\mathbf{e}^{\rm el} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.03844 & -0.01502 \\ -0.01201 & 0.08033 & 0.05363 & 0.03409 & 0.00000 & 0.00000 \\ 0.06785 & 0.06340 & 0.01872 & -0.06235 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\rm ion} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 31.95827 & -97.89358 \\ 0.56931 & 1.19393 & 2.52516 & 0.43518 & 0.00000 & 0.00000 \\ 2.15535 & 2.67582 & 3.72039 & 0.77162 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\rm tot} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 31.99671 & -97.90860 \\ 0.55730 & 1.27426 & 2.57879 & 0.46927 & 0.00000 & 0.00000 \\ 2.22320 & 2.73922 & 3.73911 & 0.70927 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 103.00429, 5.92793, 0.77088

Piezoelectric modulus: $e_m = 103.00429$ C/m^2

$TiPN_3$

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.43168 \\ 0.47848 & 0.99450 & -1.11384 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -1.04469 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & -0.34684 \\ -0.22876 & -0.60843 & 0.36036 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -0.85751 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.08484 \\ 0.24972 & 0.38607 & -0.75348 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & -1.90220 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 1.90220, 0.88269, 0.08484

Piezoelectric modulus: $e_m = 1.90220\ \mathrm{C/m^2}$

YWN_3

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.09017 & 0.42275 \\ 0.42275 & -0.42275 & 0.00000 & 0.09019 & 0.00000 & 0.00000 \\ 0.03063 & 0.03063 & -0.82535 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & -7.85798 & -4.01241 \\ -4.01241 & 4.01241 & 0.00000 & -7.85798 & 0.00000 & 0.00000 \\ -1.54897 & -1.54897 & -4.13759 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & 0.00000 & -7.76781 & -3.58966 \\ -3.58966 & 3.58966 & 0.00000 & -7.76779 & 0.00000 & 0.00000 \\ -1.51834 & -1.51834 & -4.96294 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 9.27954, 8.55713, 5.40754

Piezoelectric modulus: $e_m = 9.27954\ \mathrm{C/m^2}$

ZnP_4

$$\mathbf{e}^{\mathrm{el}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.17948 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.17948 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{ion}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.24616 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.24616 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

$$\mathbf{e}^{\mathrm{tot}} = \begin{pmatrix} 0.00000 & 0.00000 & 0.00000 & -0.42564 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.42564 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 \end{pmatrix}$$

Singular values: 0.42564, 0.42564, 0.00000

Piezoelectric modulus: $e_m = 0.42564\ \mathrm{C/m^2}$