Supplementary Information (SI) for Faraday Discussions.
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Discovery of highly anisotropic dielectric crystals with equivariant graph neural networks

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S1 AnisoNet performance on train and test splits

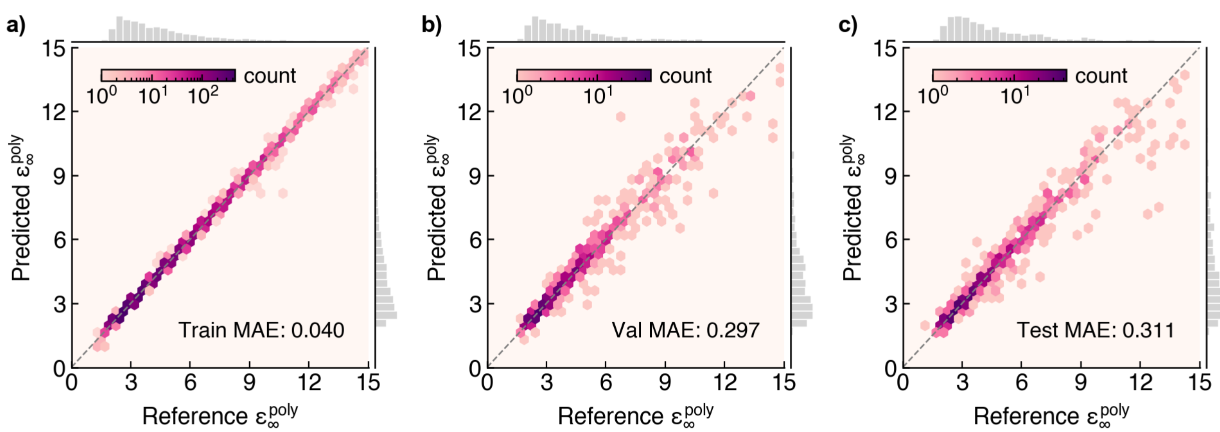

Figure S1: Performance of AnisoNet at predicting the polycrystalline dielectric constant, $\epsilon_\infty^{\mathrm{poly}}$ on the Materials Project dielectric a) train, b) validation, and c) test sets. The data is presented as heatmaps of reference vs predicted dielectric constants where a darker colour indicates more materials.

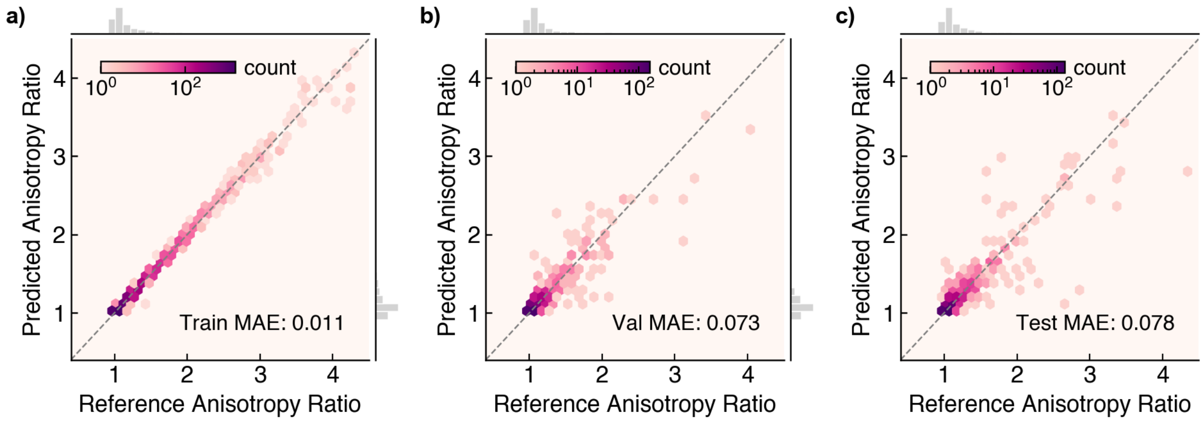

Figure S2: Performance of AnisoNet at predicting the anisotropy ratio on the Materials Project dielectric a) train, b) validation, and c) test sets. The data is presented as heatmaps of reference vs predicted dielectric constants where a darker colour indicates more materials.

S2 Analysis of predicted Materials Project dataset

While almost all materials have a predicted $\varepsilon_{\infty}^{\text{poly}}$ below 15 (the cut-off for the training set), several outliers exhibited values up to 30. The validity of these predictions should be speculated since there is no material with a higher than 15 for the model to learn from during training. The predicted anisotropy for the Materials Project dataset peaks at 1, with most predictions lying between 1 to 3 and outliers with an a_{r} up to 9.

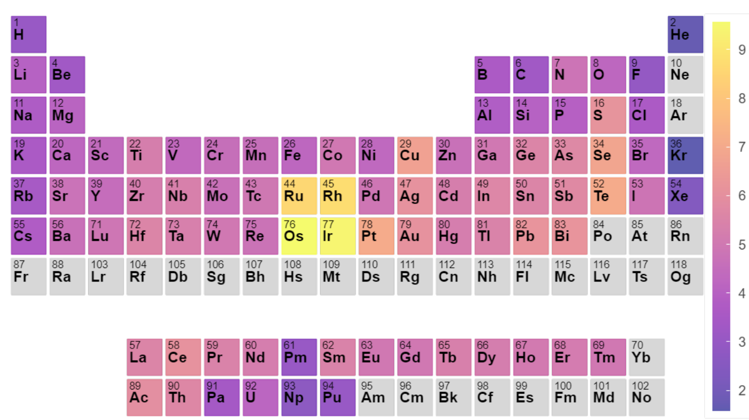

Figure S3: Average predicted polycrystalline dielectric constant ($\epsilon_{\infty}^{\text{poly}}$) of the Materials Project filtered dataset (MP-filtered) across the periodic table. Each element's colour corresponds to the average $\epsilon_{\infty}^{\text{poly}}$ for all compounds containing that element, and a brighter colour indicates a higher $\epsilon_{\infty}^{\text{poly}}$.

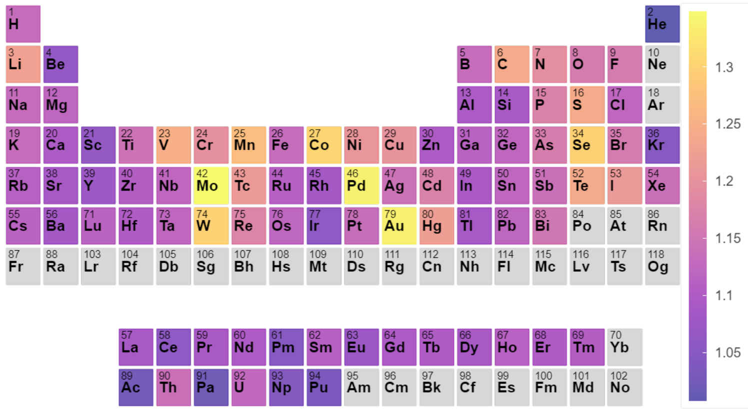

Figure S4: Average anisotropy ratio (a_r) for the MP-filtered dataset across the periodic table. Brighter colour indicates higher a_r.

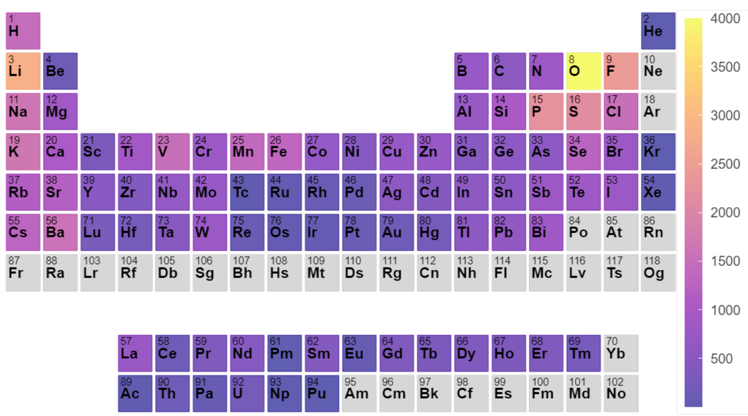

Figure S5: Number of compounds containing a certain element in the MP-filtered dataset. Note that there are 11,990 materials containing oxygen, but the colourbar is capped at 4,000 to increase the contrast between other elements.

S3 Anisotropic materials discovery

Table S1: List of materials with the highest predicted anisotropy ratio, a_r, and their DFPT-calculated dielectric tensors. *Ab initio* calculations were performed using the Vienna *ab initio* Simulation Package (VASP)[1,2] and executed using the JOBFLOW[3] and JOBFLOW-REMOTE libraries.

Material ID	Formula	Dielectric Tensor	Anisotropy Ratio
mp-1104369	NaV_2O_4	$\begin{bmatrix} 2.7 & 0.0 & -0.3 \\ 0.0 & 18.4 & 0.0 \\ -0.3 & 0.0 & 20.8 \end{bmatrix}$	7.74
mp-1313454	$LiMnCo_3O_8$	$\begin{bmatrix} 15.0 & -1.3 & 0.0 \\ -1.3 & 10.2 & 0.0 \\ 0.0 & 0.0 & 3.1 \end{bmatrix}$	5.94
mp-1023938	Te_2Mo	$\begin{bmatrix} 11.5 & 0.0 & 0.0 \\ 0.0 & 11.5 & 0.0 \\ 0.0 & 0.0 & 2.0 \end{bmatrix}$	5.63
mp-1025649	Te_6Mo_2W	$\begin{bmatrix} 12.9 & 0.0 & 0.0 \\ 0.0 & 12.9 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	5.28
mp-1025629	Te_6Mo_2W	$\begin{bmatrix} 13.1 & 0.0 & 0.0 \\ 0.0 & 13.1 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	5.24
mp-1026351	Te_6MoW_2	$\begin{bmatrix} 12.6 & 0.0 & 0.0 \\ 0.0 & 12.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	5.18

mp-1025678	Te_6MoW_2	$\begin{bmatrix} 12.6 & 0.0 & 0.0 \\ 0.0 & 12.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	5.18
mp-1025573	Te_2W	$\begin{bmatrix} 12.5 & 0.0 & 0.0 \\ 0.0 & 12.5 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	5.06
mp-1030155	Te_8Mo_3W	$\begin{bmatrix} 14.0 & 0.0 & 0.0 \\ 0.0 & 14.0 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	5.03
mp-1030331	Te_8Mo_3W	$\begin{bmatrix} 13.9 & 0.0 & 0.0 \\ 0.0 & 13.9 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	5.02
mp-1023940	$MoSe_2$	$\begin{bmatrix} 9.8 & 0.0 & 0.0 \\ 0.0 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.0 \end{bmatrix}$	5.01
mp-1030106	Te_4MoW	$\begin{bmatrix} 13.7 & 0.0 & 0.0 \\ 0.0 & 13.7 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	4.96
mp-1029256	Te_4MoW	$\begin{bmatrix} 13.7 & 0.0 & 0.0 \\ 0.0 & 13.7 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	4.96
mp-1030335	Te_4MoW	$\begin{bmatrix} 13.7 & 0.0 & 0.0 \\ 0.0 & 13.7 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	4.95

mp-1028594	Te_4MoW	$\begin{bmatrix} 13.7 & 0.0 & 0.0 \\ 0.0 & 13.7 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	4.95
mp-1023953	MoSeS	$\begin{bmatrix} 9.6 & 0.0 & 0.0 \\ 0.0 & 9.6 & 0.0 \\ 0.0 & 0.0 & 1.9 \end{bmatrix}$	4.93
mp-1028576	Te_8MoW_3	$\begin{bmatrix} 13.5 & 0.0 & 0.0 \\ 0.0 & 13.5 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	4.88
mp-1018806	MoSeS	$\begin{bmatrix} 10.7 & 0.0 & 0.0 \\ 0.0 & 10.7 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.84
mp-1030108	Te_8MoW_3	$\begin{bmatrix} 13.7 & 0.0 & 0.0 \\ 0.0 & 13.7 & 0.0 \\ 0.0 & 0.0 & 2.8 \end{bmatrix}$	4.84
mp-1025799	$MoSe_2$	$\begin{bmatrix} 11.3 & 0.0 & 0.0 \\ 0.0 & 11.3 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.82
mp-1025906	$Mo_3(Se_2S)_2$	$\begin{bmatrix} 11.0 & 0.0 & 0.0 \\ 0.0 & 11.0 & 0.0 \\ 0.0 & 0.0 & 2.3 \end{bmatrix}$	4.81
mp-1023928	$MoWSe_4$	$\begin{bmatrix} 9.5 & 0.0 & 0.0 \\ 0.0 & 9.5 & 0.0 \\ 0.0 & 0.0 & 2.0 \end{bmatrix}$	4.81

mp-1025819	$Mo_3(Se_2S)_2$	$\begin{bmatrix} 11.1 & 0.0 & 0.0 \\ 0.0 & 11.1 & 0.0 \\ 0.0 & 0.0 & 2.3 \end{bmatrix}$	4.78
mp-1025925	$Mo_3(SeS_2)_2$	$\begin{bmatrix} 10.5 & 0.0 & 0.0 \\ 0.0 & 10.5 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.76
mp-1023939	MoS_2	$\begin{bmatrix} 9.0 & 0.0 & 0.0 \\ 0.0 & 9.0 & 0.0 \\ 0.0 & 0.0 & 1.9 \end{bmatrix}$	4.75
mp-1025988	$Mo_3(SeS_2)_2$	$\begin{bmatrix} 10.8 & 0.0 & 0.0 \\ 0.0 & 10.8 & 0.0 \\ 0.0 & 0.0 & 2.3 \end{bmatrix}$	4.73
mp-1026023	$Mo_2W(SeS_2)_2$	$\begin{bmatrix} 10.0 & 0.0 & 0.0 \\ 0.0 & 10.0 & 0.0 \\ 0.0 & 0.0 & 2.1 \end{bmatrix}$	4.68
mp-1025941	$Mo_2W(SeS_2)_2$	$\begin{bmatrix} 10.1 & 0.0 & 0.0 \\ 0.0 & 10.1 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.67
mp-1025948	$Mo_2W(SeS_2)_2$	$\begin{bmatrix} 10.1 & 0.0 & 0.0 \\ 0.0 & 10.1 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.66
mp-1025874	MoS_2	$\begin{bmatrix} 10.2 & 0.0 & 0.0 \\ 0.0 & 10.2 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.64

mp-1071956	TiNF	$\begin{bmatrix} 8.8 & 0.0 & 0.0 \\ 0.0 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.1 \end{bmatrix}$	4.64
mp-1023933	WSe_2	$\begin{bmatrix} 8.6 & 0.0 & 0.0 \\ 0.0 & 8.6 & 0.0 \\ 0.0 & 0.0 & 1.9 \end{bmatrix}$	4.62
mp-1027492	MoSeS	$\begin{bmatrix} 11.6 & 0.0 & 0.0 \\ 0.0 & 11.6 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.61
mp-1027687	MoSeS	$\begin{bmatrix} 11.7 & 0.0 & 0.0 \\ 0.0 & 11.7 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.59
mp-1027795	$Mo_3W(SeS_3)_2$	$\begin{bmatrix} 10.7 & 0.0 & 0.0 \\ 0.0 & 10.7 & 0.0 \\ 0.0 & 0.0 & 2.3 \end{bmatrix}$	4.58
mp-1027580	MoSeS	$\begin{bmatrix} 11.7 & 0.0 & 0.0 \\ 0.0 & 11.7 & 0.0 \\ 0.0 & 0.0 & 2.6 \end{bmatrix}$	4.58
mp-1026980	Mo_2Se_3S	$\begin{bmatrix} 12.0 & 0.0 & 0.0 \\ 0.0 & 12.0 & 0.0 \\ 0.0 & 0.0 & 2.6 \end{bmatrix}$	4.57
mp-1026916	MoSeS	$\begin{bmatrix} 11.7 & 0.0 & 0.0 \\ 0.0 & 11.7 & 0.0 \\ 0.0 & 0.0 & 2.6 \end{bmatrix}$	4.57

mp-1027608	Mo_2SeS_3	$\begin{bmatrix} 11.4 & 0.0 & 0.0 \\ 0.0 & 11.4 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.55
mp-1025824	$MoW_2(SeS_2)_2$	$\begin{bmatrix} 9.8 & 0.0 & 0.0 \\ 0.0 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.54
mp-1027537	$Mo_3W(SeS_3)_2$	$\begin{bmatrix} 10.9 & 0.0 & 0.0 \\ 0.0 & 10.9 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.53
mp-1027890	Mo_2SeS_3	$\begin{bmatrix} 11.5 & 0.0 & 0.0 \\ 0.0 & 11.5 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.53
mp-1027472	$Mo_3W(SeS_3)_2$	$\begin{bmatrix} 10.9 & 0.0 & 0.0 \\ 0.0 & 10.9 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.53
mp-1027646	$Mo_3W(SeS_3)_2$	$\begin{bmatrix} 10.9 & 0.0 & 0.0 \\ 0.0 & 10.9 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.53
mp-1027294	$Mo_3W(SeS_3)_2$	$\begin{bmatrix} 10.9 & 0.0 & 0.0 \\ 0.0 & 10.9 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.53
mp-1025911	Mo_2WS_6	$\begin{bmatrix} 9.9 & 0.0 & 0.0 \\ 0.0 & 9.9 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.52

mp-1025663	$MoW_2(SeS_2)_2$	$\begin{bmatrix} 9.8 & 0.0 & 0.0 \\ 0.0 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.52
mp-1023929	WSeS	$\begin{bmatrix} 8.5 & 0.0 & 0.0 \\ 0.0 & 8.5 & 0.0 \\ 0.0 & 0.0 & 1.9 \end{bmatrix}$	4.52
mp-1025599	$W_3(Se_2S)_2$	$\begin{bmatrix} 9.8 & 0.0 & 0.0 \\ 0.0 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.47
mp-1025588	$W_3(Se_2S)_2$	$\begin{bmatrix} 9.8 & 0.0 & 0.0 \\ 0.0 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.46
mp-754748	CoO_2	$\begin{bmatrix} 10.8 & 0.0 & -0.1 \\ 0.0 & 10.9 & 0.1 \\ -0.1 & 0.1 & 2.4 \end{bmatrix}$	4.45
mp-1027274	$MoWSeS_3$	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.44
mp-1030745	$MoWSeS_3$	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.44
mp-1027292	$MoWSeS_3$	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.44

mp-1026975	$MoWSeS_3$	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.43
mp-1027391	$MoWSeS_3$	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.43
mp-1030146	$MoWSeS_3$	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.43
mp-1026034	$Mo(WS_3)_2$	$\begin{bmatrix} 9.6 & 0.0 & 0.0 \\ 0.0 & 9.6 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.40
mp-1027159	$MoW(SeS)_2$	$\begin{bmatrix} 11.2 & 0.0 & 0.0 \\ 0.0 & 11.2 & 0.0 \\ 0.0 & 0.0 & 2.6 \end{bmatrix}$	4.39
mp-1025689	$Mo(WS_3)_2$	$\begin{bmatrix} 9.7 & 0.0 & 0.0 \\ 0.0 & 9.7 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.39
mp-1025584	$W_3(SeS_2)_2$	$\begin{bmatrix} 9.6 & 0.0 & 0.0 \\ 0.0 & 9.6 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.39
mp-1027569	Mo_3WS_8	$\begin{bmatrix} 10.8 & 0.0 & 0.0 \\ 0.0 & 10.8 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.39

mp-1027645	Mo_3WS_8	$\begin{bmatrix} 10.8 & 0.0 & 0.0 \\ 0.0 & 10.8 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.38
mp-1025577	$W_3(SeS_2)_2$	$\begin{bmatrix} 9.8 & 0.0 & 0.0 \\ 0.0 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.3 \end{bmatrix}$	4.36
mp-1030520	$MoW_3(SeS_3)_2$	$\begin{bmatrix} 10.4 & 0.0 & 0.0 \\ 0.0 & 10.4 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.35
mp-1023925	WS_2	$\begin{bmatrix} 7.7 & 0.0 & 0.0 \\ 0.0 & 7.7 & 0.0 \\ 0.0 & 0.0 & 1.8 \end{bmatrix}$	4.35
mp-1029037	$MoW_3(SeS_3)_2$	$\begin{bmatrix} 10.4 & 0.0 & 0.0 \\ 0.0 & 10.4 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.34
mp-1028769	W_2Se_3S	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.33
mp-1028686	W_2Se_3S	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.32
mp-1030566	$MoW_3(SeS)_4$	$\begin{bmatrix} 10.9 & 0.0 & 0.0 \\ 0.0 & 10.9 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.32

mp-1027269	$MoWS_4$	$\begin{bmatrix} 10.5 & 0.0 & 0.0 \\ 0.0 & 10.5 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.31
mp-1028488	WSeS	$\begin{bmatrix} 10.4 & 0.0 & 0.0 \\ 0.0 & 10.4 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.31
mp-1028772	WSeS	$\begin{bmatrix} 10.4 & 0.0 & 0.0 \\ 0.0 & 10.4 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.30
mp-1028663	WSeS	$\begin{bmatrix} 10.4 & 0.0 & 0.0 \\ 0.0 & 10.4 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.30
mp-1027647	$MoWS_4$	$\begin{bmatrix} 10.5 & 0.0 & 0.0 \\ 0.0 & 10.5 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.30
mp-1028764	WSeS	$\begin{bmatrix} 10.4 & 0.0 & 0.0 \\ 0.0 & 10.4 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.29
mp-1030119	$MoWS_4$	$\begin{bmatrix} 10.6 & 0.0 & 0.0 \\ 0.0 & 10.6 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.29
mp-1025571	WS_2	$\begin{bmatrix} 9.3 & 0.0 & 0.0 \\ 0.0 & 9.3 & 0.0 \\ 0.0 & 0.0 & 2.2 \end{bmatrix}$	4.29

mp-1027273	MoW_3S_8	$\begin{bmatrix} 10.3 & 0.0 & 0.0 \\ 0.0 & 10.3 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.23
mp-1029246	MoW_3S_8	$\begin{bmatrix} 10.3 & 0.0 & 0.0 \\ 0.0 & 10.3 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.21
mp-1028558	W_2SeS_3	$\begin{bmatrix} 10.4 & 0.0 & 0.0 \\ 0.0 & 10.4 & 0.0 \\ 0.0 & 0.0 & 2.5 \end{bmatrix}$	4.19
mp-1278455	CoO_2	$\begin{bmatrix} 12.3 & -0.1 & -2.9 \\ -0.1 & 12.4 & -1.6 \\ -2.9 & -1.6 & 4.4 \end{bmatrix}$	4.17
mp-1028441	WS_2	$\begin{bmatrix} 10.0 & 0.0 & 0.0 \\ 0.0 & 10.0 & 0.0 \\ 0.0 & 0.0 & 2.4 \end{bmatrix}$	4.16
mp-1227328	$Ca(BC_3)_2$	$\begin{bmatrix} 14.8 & 0.0 & 0.0 \\ 0.0 & 3.7 & 0.0 \\ 0.0 & 0.0 & 13.4 \end{bmatrix}$	4.04
mp-1318786	$LiCo_3NiO_8$	$\begin{bmatrix} 12.6 & 0.4 & 0.0 \\ 0.4 & 12.3 & 0.0 \\ 0.0 & 0.0 & 3.2 \end{bmatrix}$	4.04
mp-1411545	NiS_2	$\begin{bmatrix} 7.1 & 0.0 & -2.7 \\ 0.0 & 26.6 & 0.0 \\ -2.7 & 0.0 & 26.2 \end{bmatrix}$	3.97

mp-1272680	CoO_2	$\begin{bmatrix} 11.9 & 0.0 & 0.1 \\ 0.0 & 11.9 & -0.2 \\ 0.1 & -0.2 & 3.0 \end{bmatrix}$	3.97
mp-752738	Co_3NiO_8	$\begin{bmatrix} 4.0 & -2.4 & -1.5 \\ -2.4 & 11.2 & -0.4 \\ -1.5 & -0.4 & 11.7 \end{bmatrix}$	3.96
mp-773511	Co_5NiO_{12}	$\begin{bmatrix} 12.1 & -0.1 & 0.0 \\ -0.1 & 12.0 & 0.0 \\ 0.0 & 0.0 & 3.1 \end{bmatrix}$	3.88
mp-1314136	$LiMnCo_3O_8$	$\begin{bmatrix} 5.7 & -0.5 & 3.6 \\ -0.5 & 11.2 & -0.8 \\ 3.6 & -0.8 & 8.5 \end{bmatrix}$	3.72
mp-1066781	BrCl	$\begin{bmatrix} 2.7 & 0.0 & 0.0 \\ 0.0 & 1.9 & 0.0 \\ 0.0 & 0.0 & 7.1 \end{bmatrix}$	3.65
mp-763057	$Mn(CoO_3)_2$	$\begin{bmatrix} 11.2 & 0.0 & 0.0 \\ 0.0 & 6.6 & -4.0 \\ 0.0 & -4.0 & 7.7 \end{bmatrix}$	3.59
mp-27213	$AuBr_3$	$\begin{bmatrix} 8.5 & 0.0 & 0.0 \\ 0.0 & 2.9 & 0.0 \\ 0.0 & 0.0 & 9.9 \end{bmatrix}$	3.39
mp-1296423	$LiMnCo_3O_8$	$\begin{bmatrix} 10.1 & 0.2 & 0.0 \\ 0.2 & 10.2 & 0.0 \\ 0.0 & 0.0 & 3.1 \end{bmatrix}$	3.38

mp-1285961	$Li(CoO_2)_3$	$\begin{bmatrix} 10.5 & -0.2 & -0.1 \\ -0.2 & 10.2 & 0.1 \\ -0.1 & 0.1 & 3.2 \end{bmatrix}$	3.36
mp-1303340	$LiMnCo_3O_8$	$\begin{bmatrix} 5.2 & -0.1 & 3.2 \\ -0.1 & 10.1 & 0.0 \\ 3.2 & 0.0 & 7.7 \end{bmatrix}$	3.34
mp-755555	Mn_5CoO_{12}	$\begin{bmatrix} 9.8 & -0.1 & 0.0 \\ -0.1 & 9.8 & 0.0 \\ 0.0 & 0.0 & 2.9 \end{bmatrix}$	3.34
mp-755862	$LiMnCo_3O_8$	$\begin{bmatrix} 5.1 & -0.1 & 3.1 \\ -0.1 & 9.5 & -0.1 \\ 3.1 & -0.1 & 7.6 \end{bmatrix}$	3.22
mp-1184859	HI_3	$\begin{bmatrix} 3.0 & -1.8 & 0.0 \\ -1.8 & 4.6 & 0.0 \\ 0.0 & 0.0 & 1.8 \end{bmatrix}$	3.21
mp-759301	$Li(CoO_2)_3$	$\begin{bmatrix} 10.6 & 0.1 & 0.0 \\ 0.1 & 10.7 & 0.0 \\ 0.0 & 0.0 & 3.4 \end{bmatrix}$	3.12
mp-759163	VOF_2	$\begin{bmatrix} 3.2 & 0.0 & 0.0 \\ 0.0 & 7.9 & -3.2 \\ 0.0 & -3.2 & 5.5 \end{bmatrix}$	3.12
mp-1217314	$TeMo_2Se_3$	$\begin{bmatrix} 16.4 & 0.0 & 0.0 \\ 0.0 & 16.4 & 0.0 \\ 0.0 & 0.0 & 5.3 \end{bmatrix}$	3.09

mp-1018809	MoS_2	$\begin{bmatrix} 14.3 & 0.0 & 0.0 \\ 0.0 & 14.3 & 0.0 \\ 0.0 & 0.0 & 4.7 \end{bmatrix}$	3.03
mp-1221404	MoSeS	$\begin{bmatrix} 15.0 & 0.0 & 0.0 \\ 0.0 & 15.0 & 0.0 \\ 0.0 & 0.0 & 5.0 \end{bmatrix}$	3.02
mp-9481	TcS_2	$\begin{bmatrix} 15.6 & -1.2 & 2.0 \\ -1.2 & 14.2 & 3.8 \\ 2.0 & 3.8 & 7.7 \end{bmatrix}$	2.99
mp-572758	ReS_2	$\begin{bmatrix} 14.0 & -0.2 & 0.0 \\ -0.2 & 12.7 & 2.0 \\ 0.0 & 2.0 & 5.3 \end{bmatrix}$	2.96
mp-1217371	Te_3Mo_2Se	$\begin{bmatrix} 17.9 & 0.0 & 0.0 \\ 0.0 & 17.9 & 0.0 \\ 0.0 & 0.0 & 6.0 \end{bmatrix}$	2.96
mp-754774	$Li_2Mn_3(CoO_4)_3$	$\begin{bmatrix} 8.9 & 0.1 & -0.1 \\ 0.1 & 4.8 & -2.6 \\ -0.1 & -2.6 & 7.1 \end{bmatrix}$	2.93
mp-1018807	$MoSe_2$	$\begin{bmatrix} 15.7 & 0.0 & 0.0 \\ 0.0 & 15.7 & 0.0 \\ 0.0 & 0.0 & 5.5 \end{bmatrix}$	2.86
mp-1219546	ReSeS	$\begin{bmatrix} 6.1 & -2.8 & 0.0 \\ -2.8 & 13.0 & -0.5 \\ 0.0 & -0.5 & 14.3 \end{bmatrix}$	2.84

mp-1221485	Mo_2SeS_3	$\begin{bmatrix} 15.0 & 0.0 & 0.0 \\ 0.0 & 15.0 & 0.0 \\ 0.0 & 0.0 & 5.4 \end{bmatrix}$	2.80
mp-753228	$LiMn_3O_6$	$\begin{bmatrix} 8.2 & 0.0 & 0.0 \\ 0.0 & 7.6 & -0.1 \\ 0.0 & -0.1 & 3.1 \end{bmatrix}$	2.62
mp-1276496	NaV_2O_4	$\begin{bmatrix} 2.7 & 0.0 & 0.1 \\ 0.0 & 5.4 & 0.1 \\ 0.1 & 0.1 & 7.0 \end{bmatrix}$	2.62
mp-861871	SeI_2	$\begin{bmatrix} 5.0 & 0.0 & 0.0 \\ 0.0 & 5.0 & 0.0 \\ 0.0 & 0.0 & 13.0 \end{bmatrix}$	2.58
mp-752885	$LiVOF_3$	$\begin{bmatrix} 3.2 & -0.8 & -0.9 \\ -0.8 & 4.6 & 1.8 \\ -0.9 & 1.8 & 4.9 \end{bmatrix}$	2.53
mp-756552	$Mg(NiO_2)_4$	$\begin{bmatrix} 8.9 & 0.0 & 0.0 \\ 0.0 & 8.9 & 0.0 \\ 0.0 & 0.0 & 3.6 \end{bmatrix}$	2.51
mp-1016190	KMn_3O_6	$\begin{bmatrix} 6.0 & 0.0 & 0.0 \\ 0.0 & 2.4 & 0.0 \\ 0.0 & 0.0 & 5.5 \end{bmatrix}$	2.49
mp-1273655	MnOF	$\begin{bmatrix} 4.0 & -0.6 & 0.1 \\ -0.6 & 6.0 & 0.9 \\ 0.1 & 0.9 & 2.9 \end{bmatrix}$	2.43

mp-1223545	KMn_2O_4	$\begin{bmatrix} 2.8 & 0.0 & 0.2 \\ 0.0 & 6.7 & 0.0 \\ 0.2 & 0.0 & 5.9 \end{bmatrix}$	2.42
mp-997108	$RbAgO_2$	$\begin{bmatrix} 4.6 & -1.4 & -0.6 \\ -1.4 & 4.0 & 0.1 \\ -0.6 & 0.1 & 2.7 \end{bmatrix}$	2.42
mp-2422143	$Pd(Se_3Br)_2$	$\begin{bmatrix} 3.8 & 0.0 & -0.2 \\ 0.0 & 6.9 & -1.5 \\ -0.2 & -1.5 & 8.3 \end{bmatrix}$	2.42
mp-1104174	$K_4(NiO_2)_3$	$\begin{bmatrix} 2.7 & 0.0 & 0.4 \\ 0.0 & 3.4 & 0.0 \\ 0.4 & 0.0 & 1.6 \end{bmatrix}$	2.41
mp-1101129	$ThPbI_{12}$	$\begin{bmatrix} 7.6 & 0.0 & 0.0 \\ 0.0 & 4.1 & 0.0 \\ 0.0 & 0.0 & 3.2 \end{bmatrix}$	2.37
mp-1018888	$PdCl_2$	$\begin{bmatrix} 5.6 & 0.0 & 0.0 \\ 0.0 & 2.4 & 0.2 \\ 0.0 & 0.2 & 3.4 \end{bmatrix}$	2.33
mp-1003484	$MgMn_4O_8$	$\begin{bmatrix} 6.7 & 0.2 & 1.0 \\ 0.2 & 7.7 & -0.8 \\ 1.0 & -0.8 & 3.9 \end{bmatrix}$	2.31
mp-758725	$Li_2(CoO_2)_3$	$\begin{bmatrix} 9.1 & 0.0 & 0.0 \\ 0.0 & 9.1 & 0.0 \\ 0.0 & 0.0 & 4.0 \end{bmatrix}$	2.31

mp-1068977	K_2PdC_2	$\begin{bmatrix} 3.6 & 0.0 & 0.0 \\ 0.0 & 3.6 & 0.0 \\ 0.0 & 0.0 & 8.1 \end{bmatrix}$	2.29
mp-20343	$NaAuO_2$	$\begin{bmatrix} 2.8 & 0.0 & 0.0 \\ 0.0 & 3.5 & 0.0 \\ 0.0 & 0.0 & 6.2 \end{bmatrix}$	2.25
mp-3342	$ZnPS_3$	$\begin{bmatrix} 6.8 & 0.0 & 0.0 \\ 0.0 & 6.8 & 0.0 \\ 0.0 & 0.0 & 3.3 \end{bmatrix}$	2.04
mp-772788	$Ba_2Cu_2O_5$	$\begin{bmatrix} 4.1 & 0.0 & 0.0 \\ 0.0 & 8.0 & 0.0 \\ 0.0 & 0.0 & 5.8 \end{bmatrix}$	1.97
mp-1193708	$Al_2(PS_3)_3$	$\begin{bmatrix} 6.5 & 0.0 & 0.0 \\ 0.0 & 6.5 & 0.0 \\ 0.0 & 0.0 & 3.5 \end{bmatrix}$	1.88
mp-569017	PdI_2	$\begin{bmatrix} 12.8 & 0.0 & 0.0 \\ 0.0 & 7.0 & 0.0 \\ 0.0 & 0.0 & 7.8 \end{bmatrix}$	1.82
mp-580886	ZrIN	$\begin{bmatrix} 5.6 & 0.0 & -0.2 \\ 0.0 & 7.9 & 0.0 \\ -0.2 & 0.0 & 7.9 \end{bmatrix}$	1.42
mp-567441	HfIN	$\begin{bmatrix} 5.4 & 0.0 & -0.2 \\ 0.0 & 7.2 & 0.0 \\ -0.2 & 0.0 & 7.2 \end{bmatrix}$	1.34

mp-561973	$K(TeO_3)_2$	$\begin{bmatrix} 4.4 & 0.0 & 0.0 \\ 0.0 & 4.0 & 0.2 \\ 0.0 & 0.2 & 4.5 \end{bmatrix}$	1.16

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