Benchmark Score Table

Model	Avg MAE ↓	Rank
mace_omat_0_D3	5.335	1
mace_matpes_r2scan_0_D3	5.391	2
mace_mpa_0_D3	6.422	3
mace_mp_0a_D3	9.446	4
mace_matpes_PBE_0_D3	9.703	5
mace_mp_0b3_D3	11.553	6

Combined MAE Table

Model	K_{bulk} [GPa]	K_{shear} [GPa]	Elasticity Score (avg)	Rank	Lat Const [Å]	Rank	ω_{max} [THz]	S [J/mol · K]	F [kJ/mol]	C_V [J/mol · K]	Phonon Score (avg)	Rank
mace_mp_0a_D3	43.032	13.867	30.95	4	0.027	2	0.631	4.63	1.42	0.101	1.696	6
mace_mp_0b3_D3	56.672	23.4	40.036	6	0.027	2	0.38	3.637	1.113	0.073	1.301	4
mace_mpa_0_D3	13.211	3.442	22.326	3	0.019	1	0.025	2.44	0.745	0.041	0.813	2
mace_omat_0_D3	22.798	11.507	17.152	2	0.067	6	0.002	2.116	0.646	0.037	0.7	1
mace_matpes_PBE_0_D3	47.355	26.274	31.914	5	0.035	4	0.476	3.658	1.12	0.075	1.332	5
mace_matpes_r2scan_0_D3	32.493	16.101	16.797	1	0.044	5	0.008	3.169	0.97	0.063	1.052	3

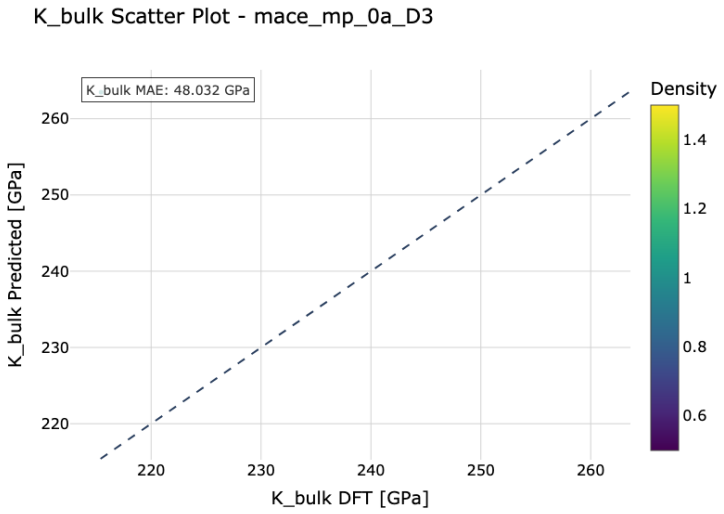
Elasticity Report

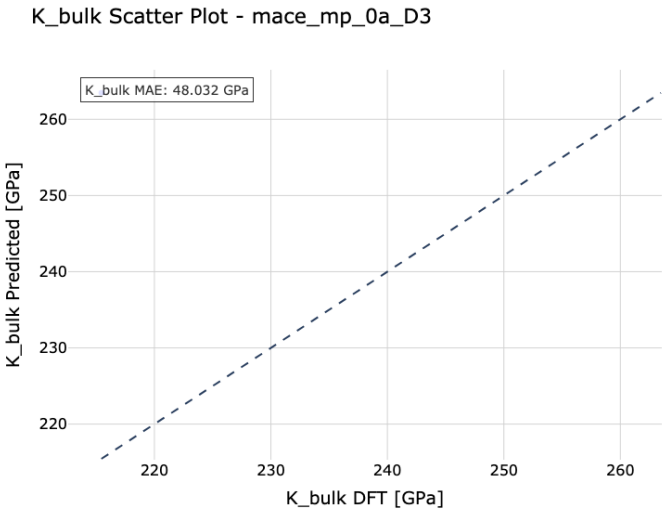
Bulk and Shear Moduli MAE Table

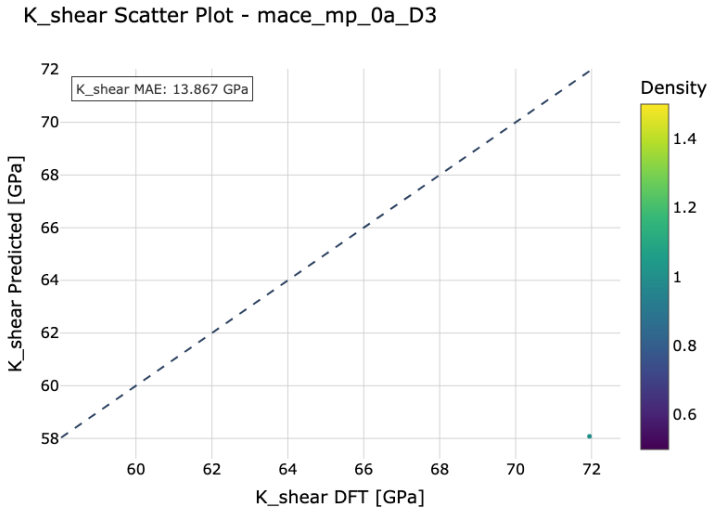
Model	K_bulk [GPa]	K_shear [GPa]	Elasticity Score (avg)	Rank
mace_mp_0a_D3	48.032	13.867	30.95	4
mace_mp_0b3_D3	56.672	23.4	40.036	6
mace_mpa_0_D3	41.211	3.442	22.326	3
mace_omat_0_D3	22.798	11.507	17.152	2
mace_matpes_PBE_0_D3	47.555	16.274	31.914	5
mace_matpes_r2scan_0_D3	30.493	3.101	16.797	1

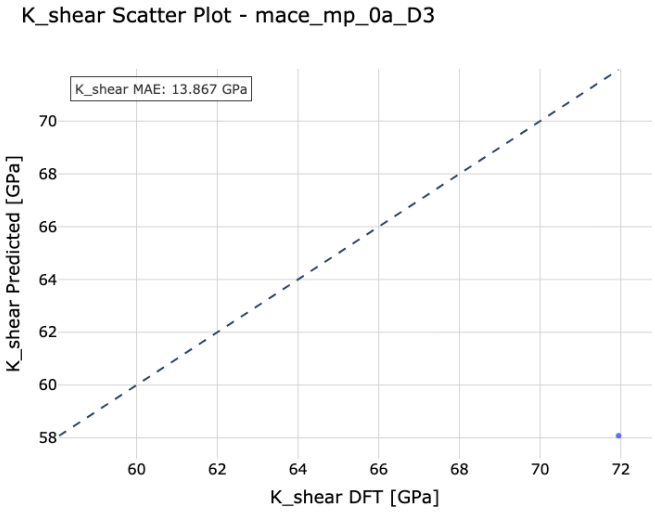
Scatter and density Plots

mace_mp_0a_D3

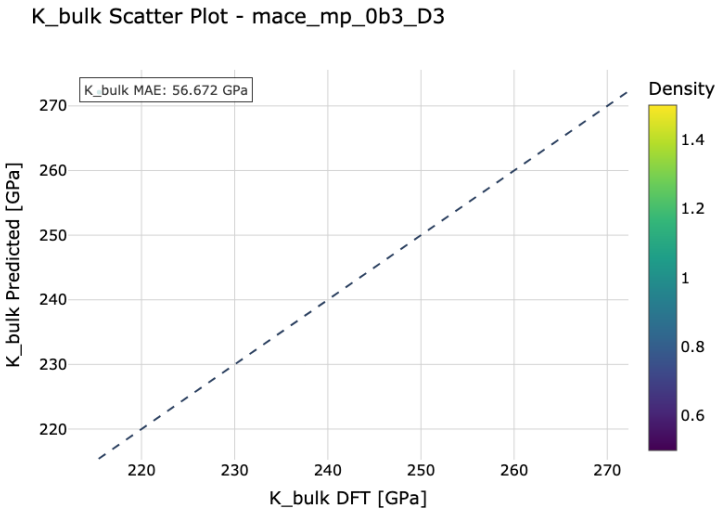


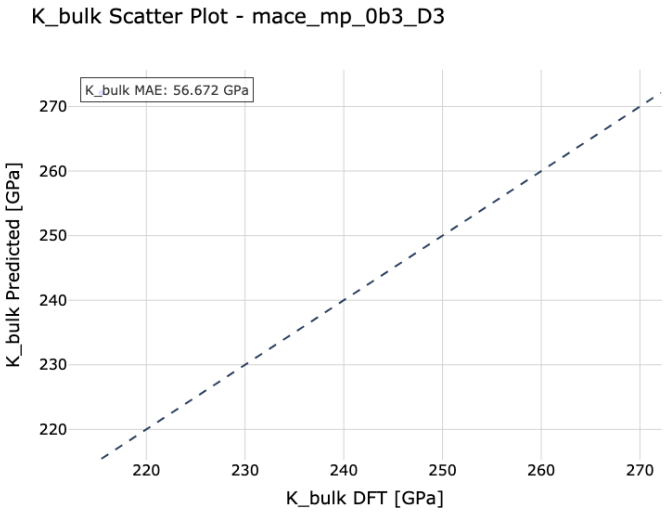


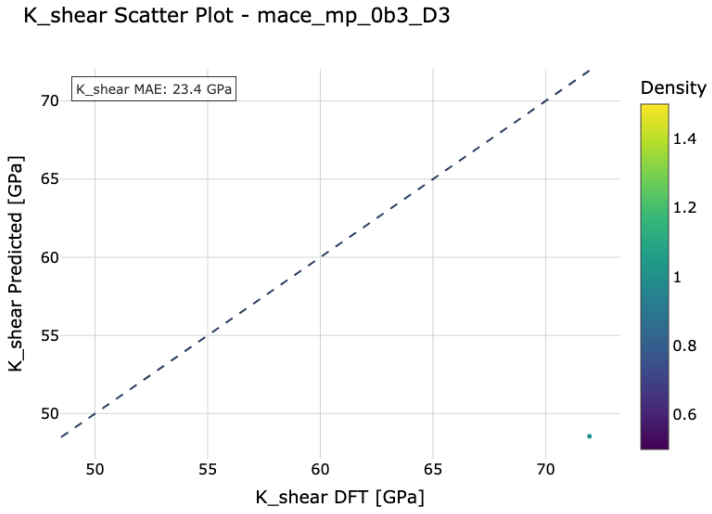


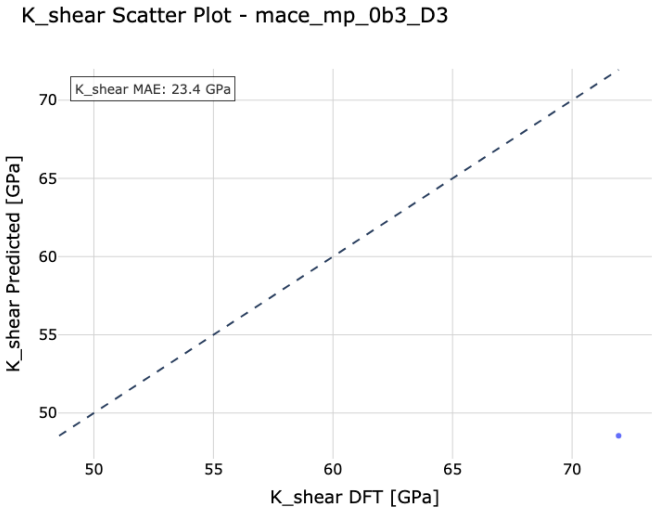


mace_mp_0b3_D3

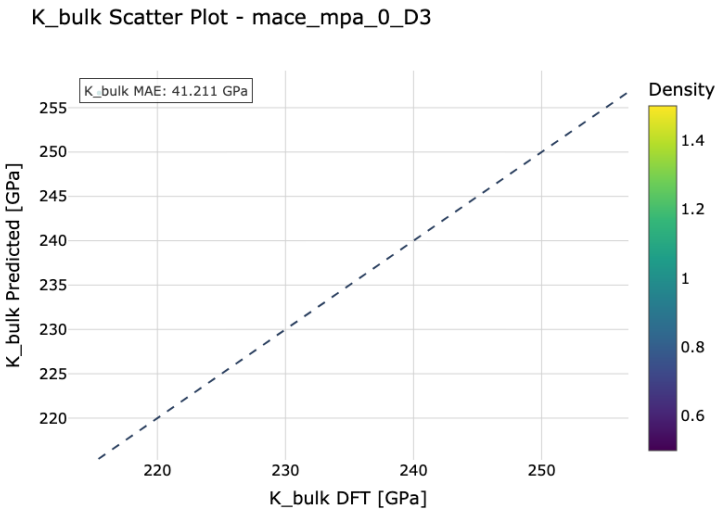


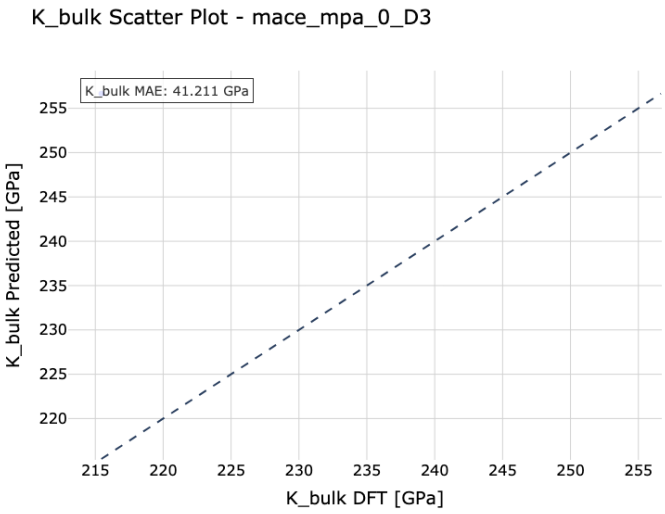


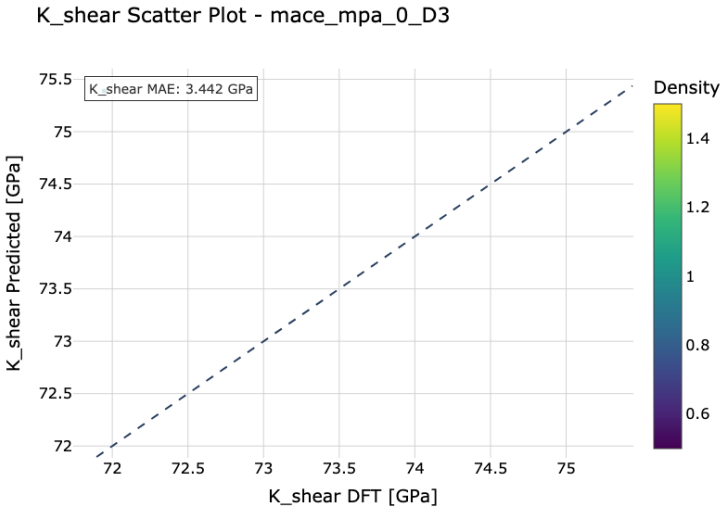


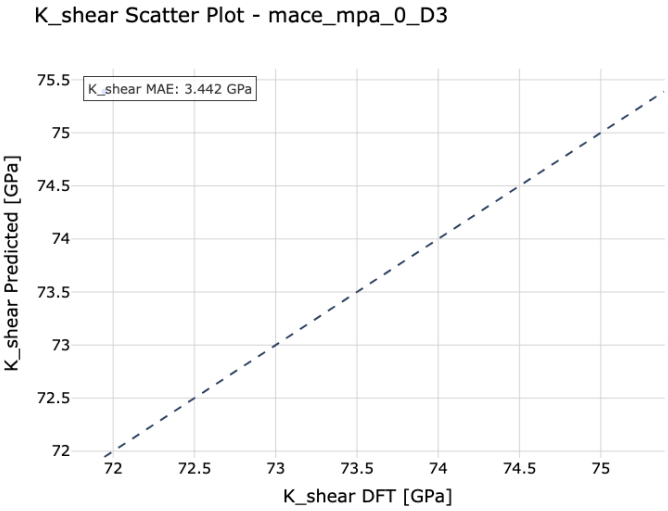


mace_mpa_0_D3

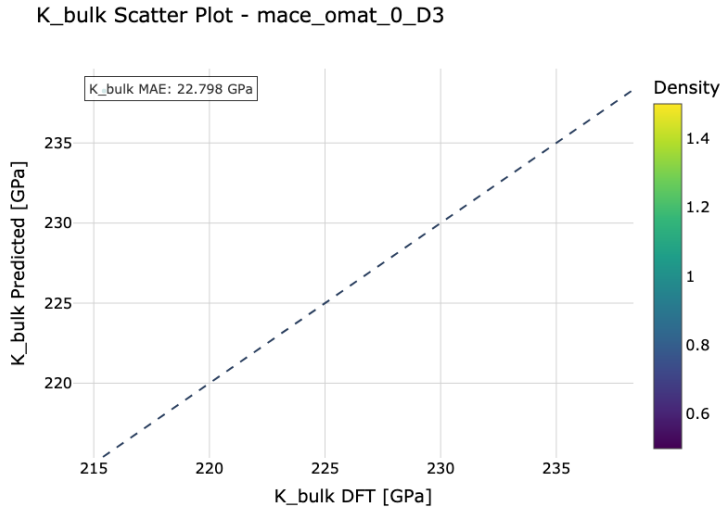


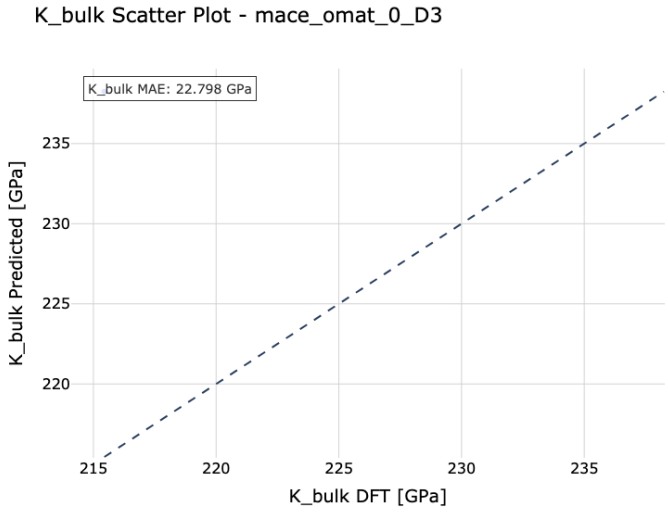


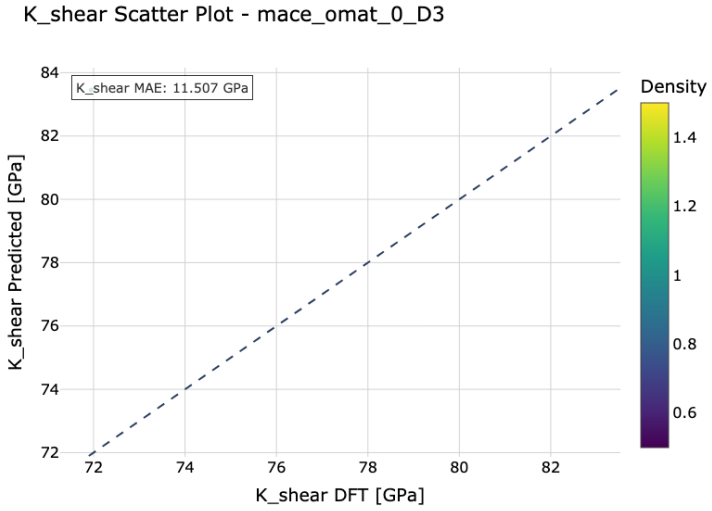


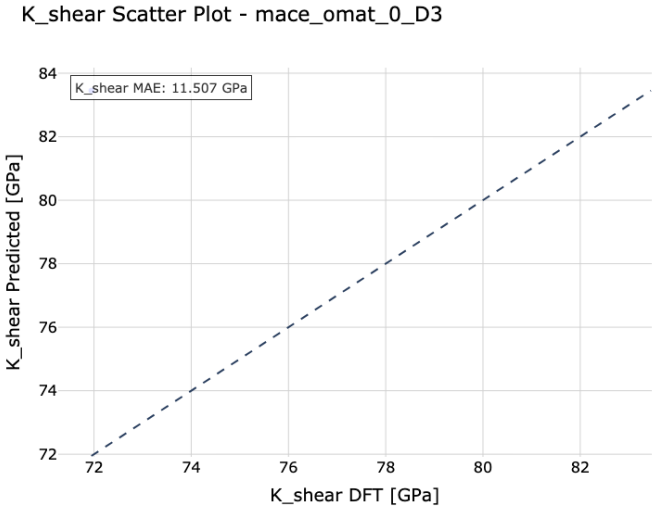


mace_omat_0_D3

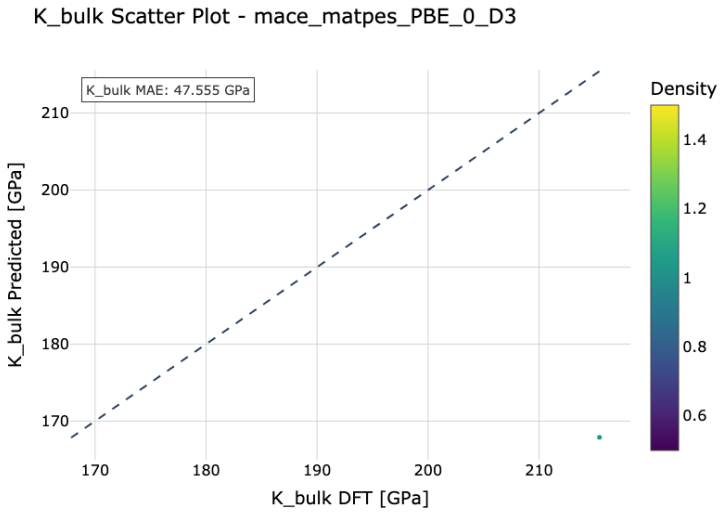


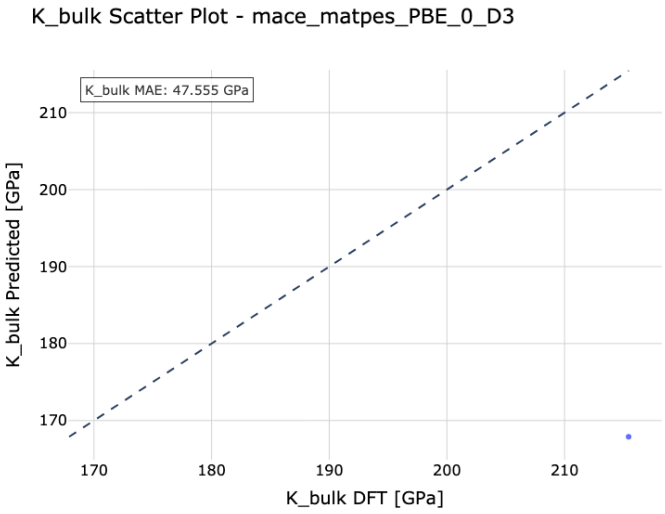


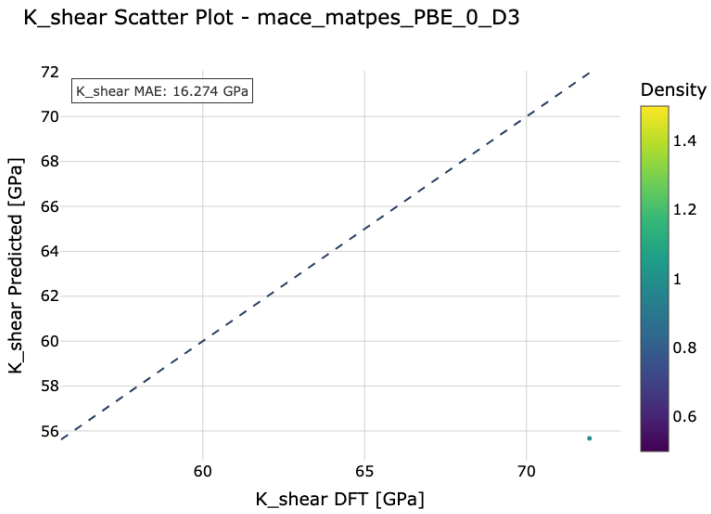


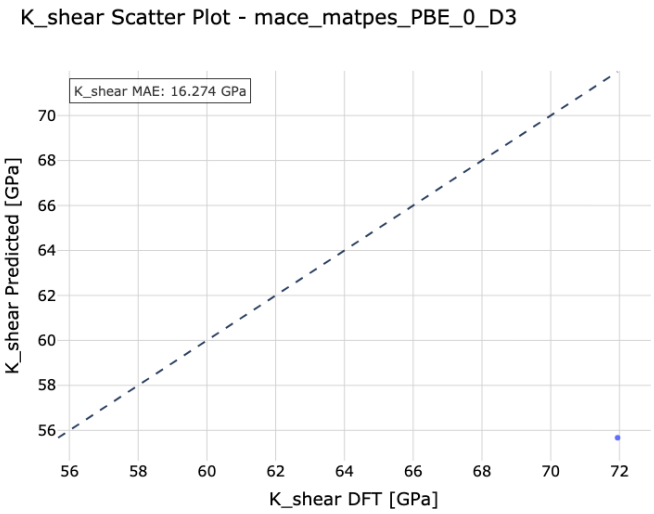


mace_matpes_PBE_0_D3

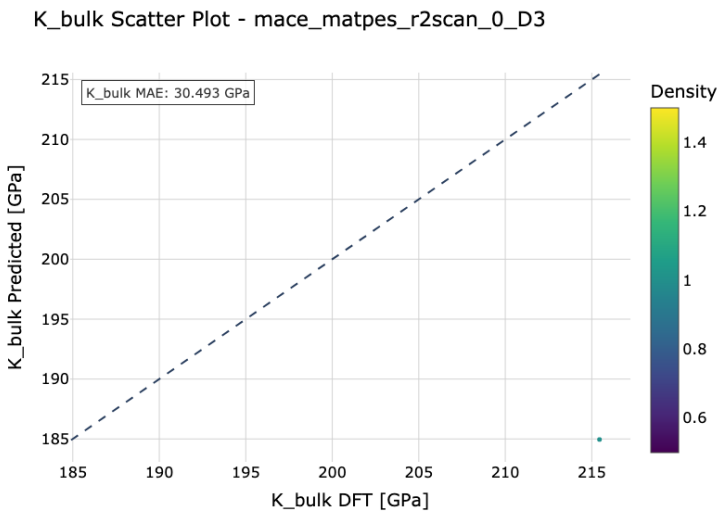


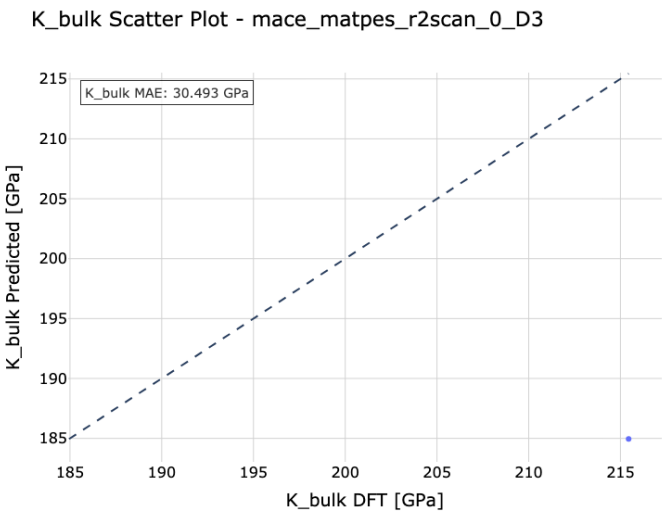


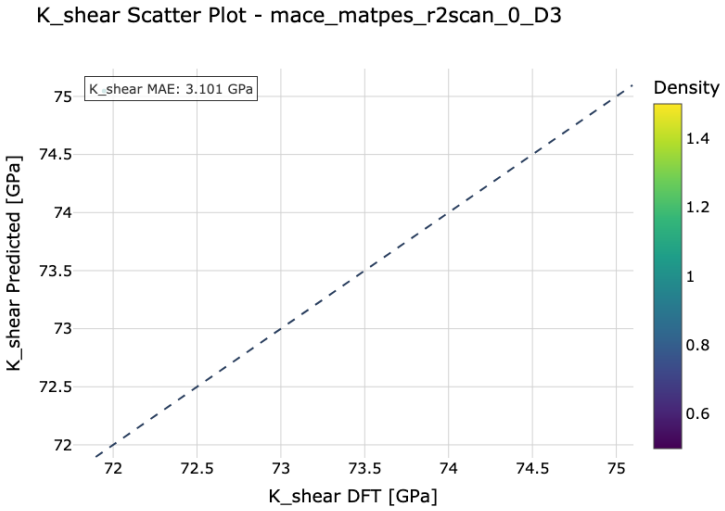


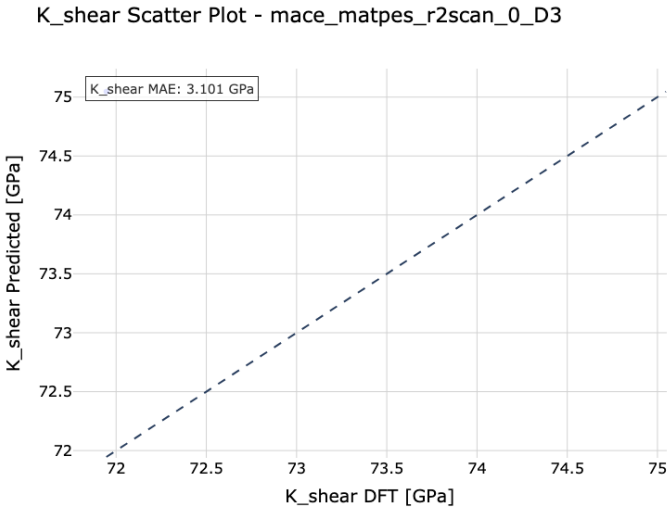


mace_matpes_r2scan_0_D3






K_shear Scatter Plot - mace_matpes_r2scan_0_D3
K_shear MAE: 3.101 GPa
Density
1.4
1.2
1
0.8
0.6
K_shear Predicted [GPa]
K_shear DFT [GPa]
72
72.5
73
73.5
74
74.5
75


K_shear Scatter Plot - mace_matpes_r2scan_0_D3
K_shear MAE: 3.101 GPa
K_shear Predicted [GPa]
K_shear DFT [GPa]
72
72.5
73
73.5
74
74.5
75

Lattice Constants Report

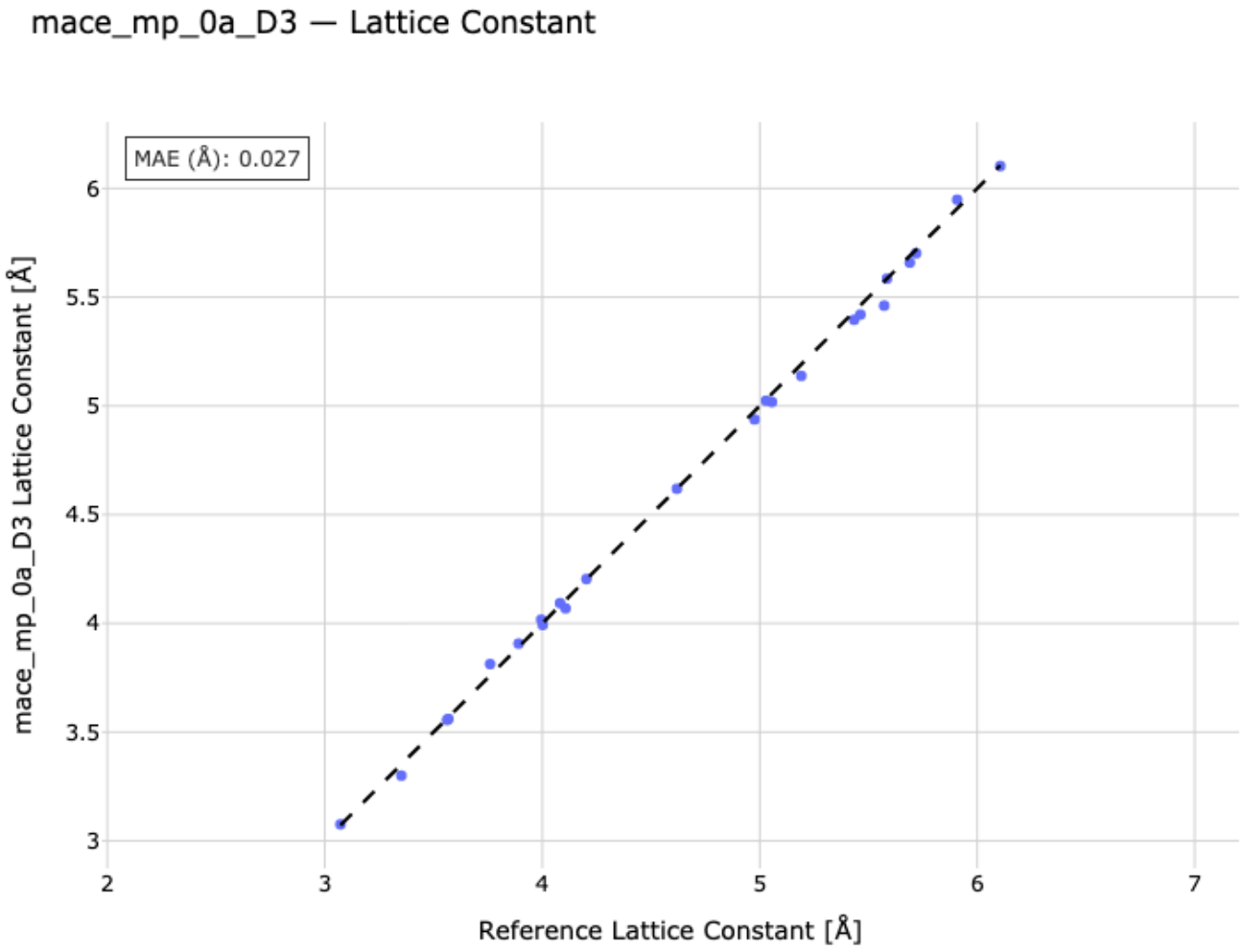
Lattice Constants MAE Table

Model	Lat Const [Å]	Rank
mace_mp_0a_D3	0.027	2
mace_mp_0b3_D3	0.027	2
mace_mpa_0_D3	0.019	1
mace_omat_0_D3	0.067	6
mace_matpes_PBE_0_D3	0.035	4
mace_matpes_r2scan_0_D3	0.044	5

Per-Model Tables and Scatter Plots

mace_mp_0a_D3

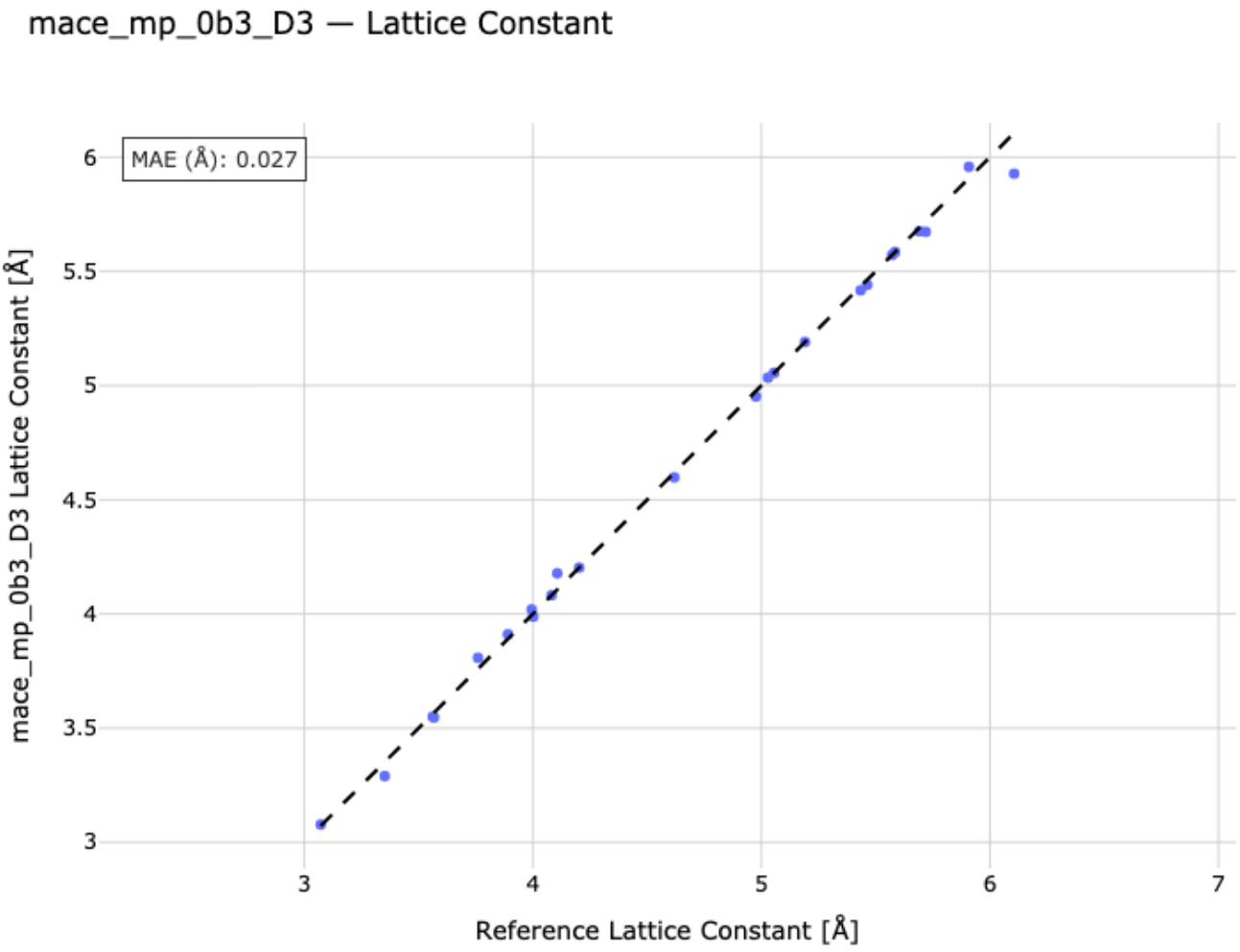
Element	DFT (Å)	mace_mp_0a_D3 (Å)	Δ	Δ/%
Ag	4.082	4.093	0.011	0.27
Pd	3.891	3.907	0.016	0.41
Rh	3.76	3.813	0.053	1.41
Li	3.352	3.3	-0.052	-1.55
Na	4.107	4.069	-0.038	-0.93
K	5.191	5.138	-0.053	-1.02
Rb	5.572	5.461	-0.111	-1.99
Cs	6.106	6.103	-0.003	-0.05
Ca	5.463	5.42	-0.043	-0.79
Sr	5.908	5.948	0.04	0.68
Ba	4.976	4.938	-0.038	-0.76
Al	4.002	3.993	-0.009	-0.22
LiF	3.995	4.017	0.022	0.55
NaF	4.619	4.619	0	0
NaCl	5.585	5.585	0	0
MgO	4.203	4.204	0.001	0.02
Si	5.434	5.396	-0.038	-0.7
Ge	5.719	5.702	-0.017	-0.3
GaAs	5.69	5.659	-0.031	-0.54
Cu	3.568	3.561	-0.007	-0.2
C	3.562	3.556	-0.006	-0.17
LiCl	5.056	5.018	-0.038	-0.75
SiC(a)	3.072	3.076	0.004	0.13
SiC(c)	5.029	5.024	-0.005	-0.1



mace__mp__0b3__D3

Element	DFT (Å)	mace__mp__0b3__D3 (Å)	Δ	Δ/%
Ag	4.082	4.082	0	0
Pd	3.891	3.911	0.02	0.51
Rh	3.76	3.808	0.048	1.28
Li	3.352	3.29	-0.062	-1.85
Na	4.107	4.178	0.071	1.73
K	5.191	5.191	0	0
Rb	5.572	5.572	0	0
Cs	6.106	5.928	-0.178	-2.92
Ca	5.463	5.441	-0.022	-0.4
Sr	5.908	5.958	0.05	0.85
Ba	4.976	4.952	-0.024	-0.48
Al	4.002	3.988	-0.014	-0.35
LiF	3.995	4.02	0.025	0.63
NaF	4.619	4.598	-0.021	-0.45
NaCl	5.585	5.585	0	0
MgO	4.203	4.203	0	0
Si	5.434	5.417	-0.017	-0.31
Ge	5.719	5.673	-0.046	-0.8

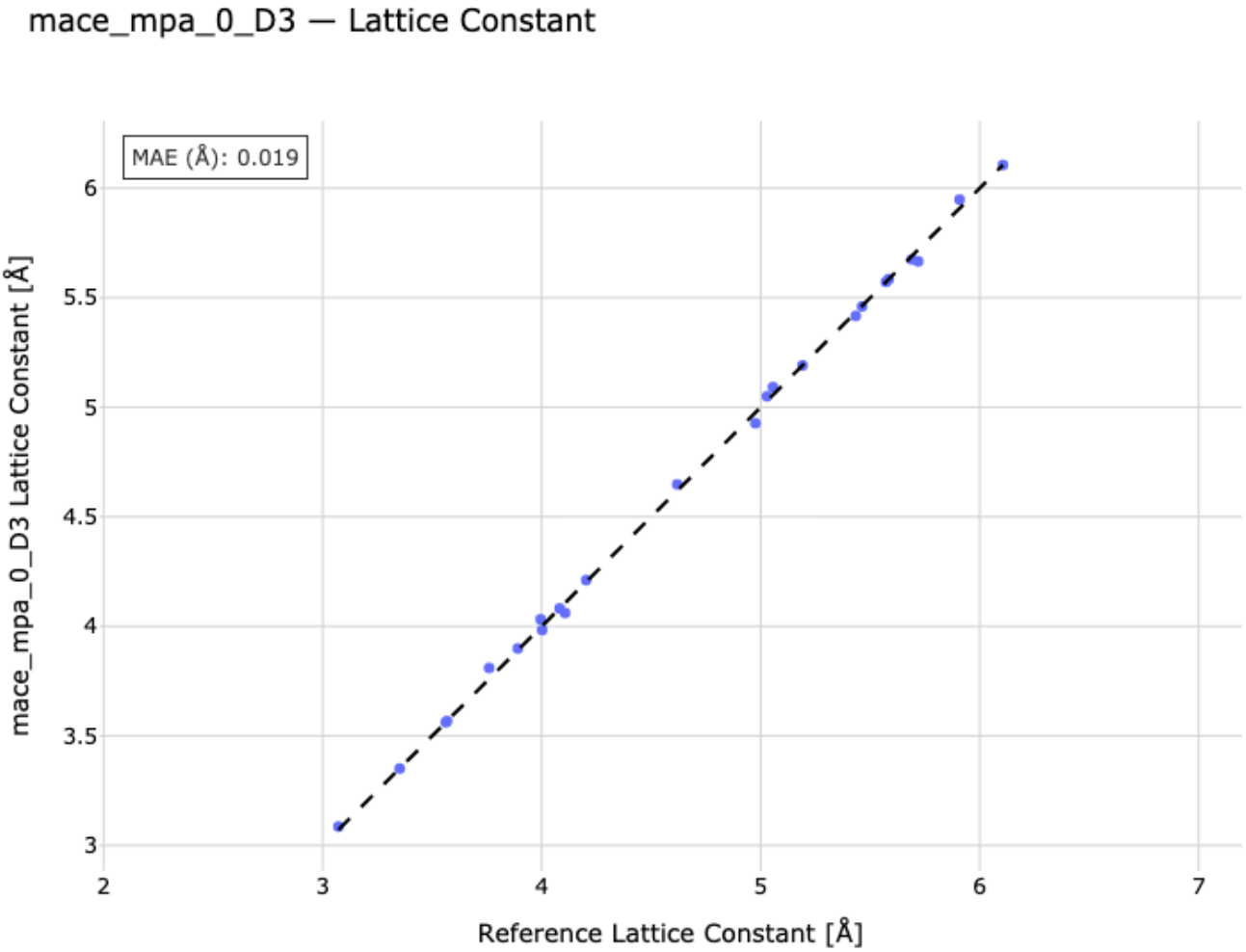
Element	DFT (Å)	mace_mp_0b3_D3 (Å)	Δ	Δ/%
GaAs	5.69	5.676	-0.014	-0.25
Cu	3.568	3.547	-0.021	-0.59
C	3.562	3.55	-0.012	-0.34
LiCl	5.056	5.056	0	0
SiC(a)	3.072	3.078	0.006	0.2
SiC(c)	5.029	5.035	0.006	0.12



mace_mpa_0_D3

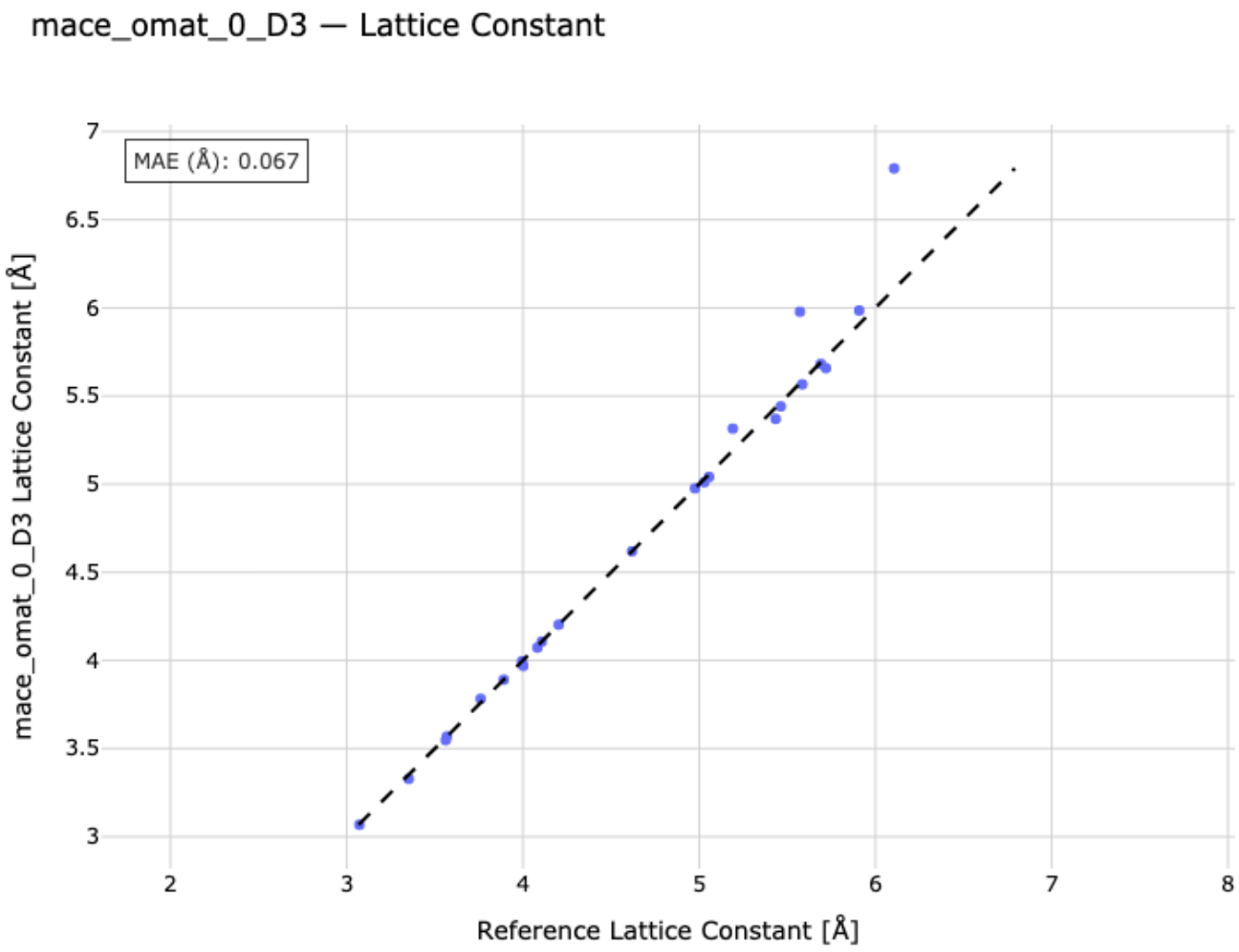
Element	DFT (Å)	mace_mpa_0_D3 (Å)	Δ	Δ/%
Ag	4.082	4.082	0	0
Pd	3.891	3.899	0.008	0.21
Rh	3.76	3.81	0.05	1.33
Li	3.352	3.351	-0.001	-0.03
Na	4.107	4.061	-0.046	-1.12
K	5.191	5.191	0	0
Rb	5.572	5.572	0	0
Cs	6.106	6.106	0	0

Element	DFT (Å)	mace_mpa_0_D3 (Å)	Δ	Δ/%
Ca	5.463	5.46	-0.003	-0.05
Sr	5.908	5.948	0.04	0.68
Ba	4.976	4.927	-0.049	-0.98
Al	4.002	3.983	-0.019	-0.47
LiF	3.995	4.032	0.037	0.93
NaF	4.619	4.648	0.029	0.63
NaCl	5.585	5.585	0	0
MgO	4.203	4.211	0.008	0.19
Si	5.434	5.417	-0.017	-0.31
Ge	5.719	5.666	-0.053	-0.93
GaAs	5.69	5.675	-0.015	-0.26
Cu	3.568	3.568	0	0
C	3.562	3.562	0	0
LiCl	5.056	5.092	0.036	0.71
SiC(a)	3.072	3.086	0.014	0.46
SiC(c)	5.029	5.05	0.021	0.42



mace_omat_0_D3

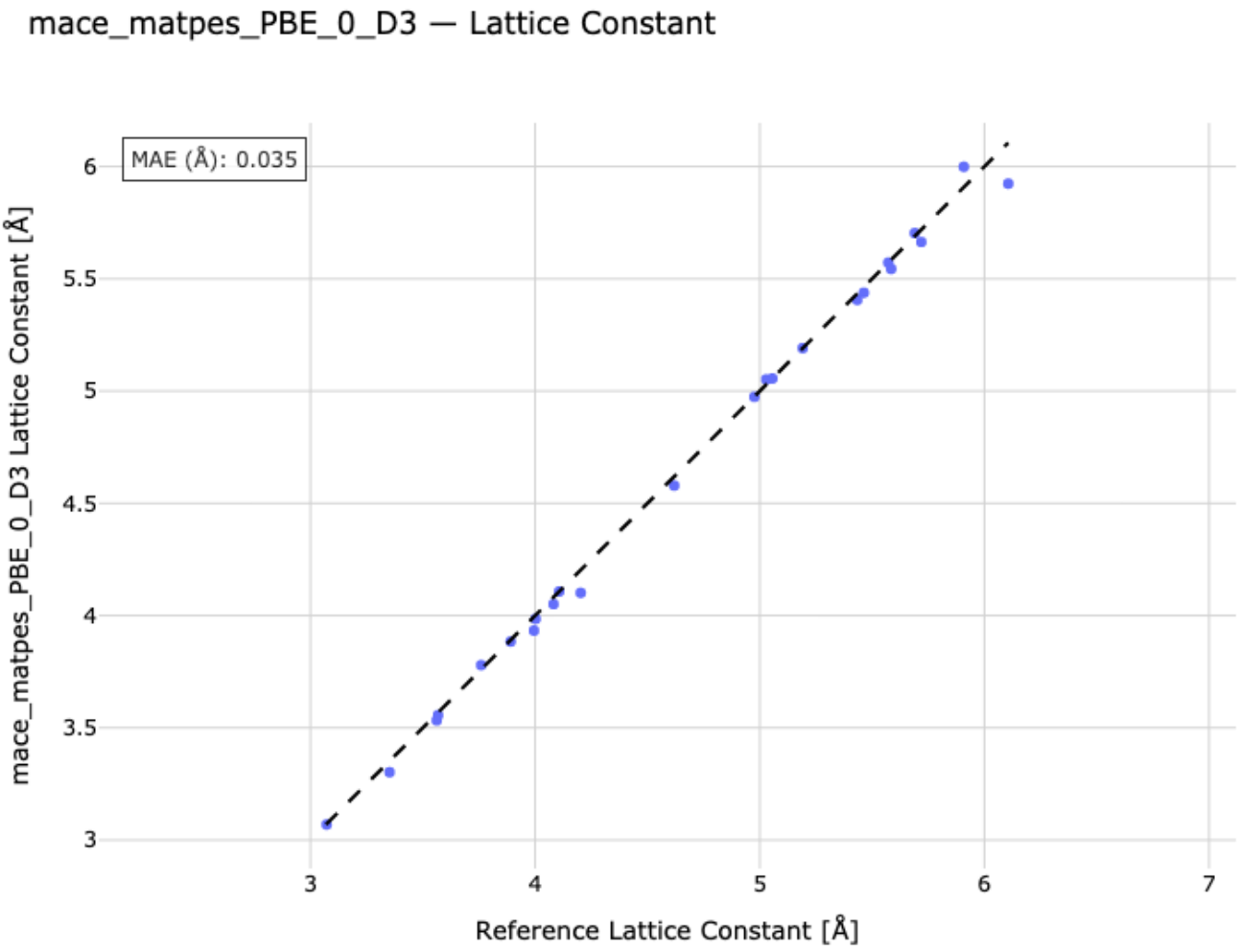
Element	DFT (Å)	mace_omat_0_D3 (Å)	Δ	Δ/%
Ag	4.082	4.073	-0.009	-0.22
Pd	3.891	3.891	0	0
Rh	3.76	3.782	0.022	0.59
Li	3.352	3.328	-0.024	-0.72
Na	4.107	4.107	0	0
K	5.191	5.315	0.124	2.39
Rb	5.572	5.978	0.406	7.29
Cs	6.106	6.791	0.685	11.22
Ca	5.463	5.441	-0.022	-0.4
Sr	5.908	5.985	0.077	1.3
Ba	4.976	4.976	0	0
Al	4.002	3.969	-0.033	-0.82
LiF	3.995	3.995	0	0
NaF	4.619	4.619	0	0
NaCl	5.585	5.566	-0.019	-0.34
MgO	4.203	4.203	0	0
Si	5.434	5.37	-0.064	-1.18
Ge	5.719	5.658	-0.061	-1.07
GaAs	5.69	5.682	-0.008	-0.14
Cu	3.568	3.568	0	0
C	3.562	3.548	-0.014	-0.39
LiCl	5.056	5.041	-0.015	-0.3
SiC(a)	3.072	3.068	-0.004	-0.13
SiC(c)	5.029	5.011	-0.018	-0.36



mace_matpes_PBE_0_D3

Element	DFT (Å)	mace_matpes_PBE_0_D3 (Å)	Δ	Δ/%
Ag	4.082	4.051	-0.031	-0.76
Pd	3.891	3.884	-0.007	-0.18
Rh	3.76	3.779	0.019	0.51
Li	3.352	3.302	-0.05	-1.49
Na	4.107	4.107	0	0
K	5.191	5.191	0	0
Rb	5.572	5.572	0	0
Cs	6.106	5.924	-0.182	-2.98
Ca	5.463	5.438	-0.025	-0.46
Sr	5.908	5.999	0.091	1.54
Ba	4.976	4.974	-0.002	-0.04
Al	4.002	3.985	-0.017	-0.42
LiF	3.995	3.933	-0.062	-1.55
NaF	4.619	4.579	-0.04	-0.87
NaCl	5.585	5.544	-0.041	-0.73
MgO	4.203	4.101	-0.102	-2.43
Si	5.434	5.406	-0.028	-0.52
Ge	5.719	5.664	-0.055	-0.96

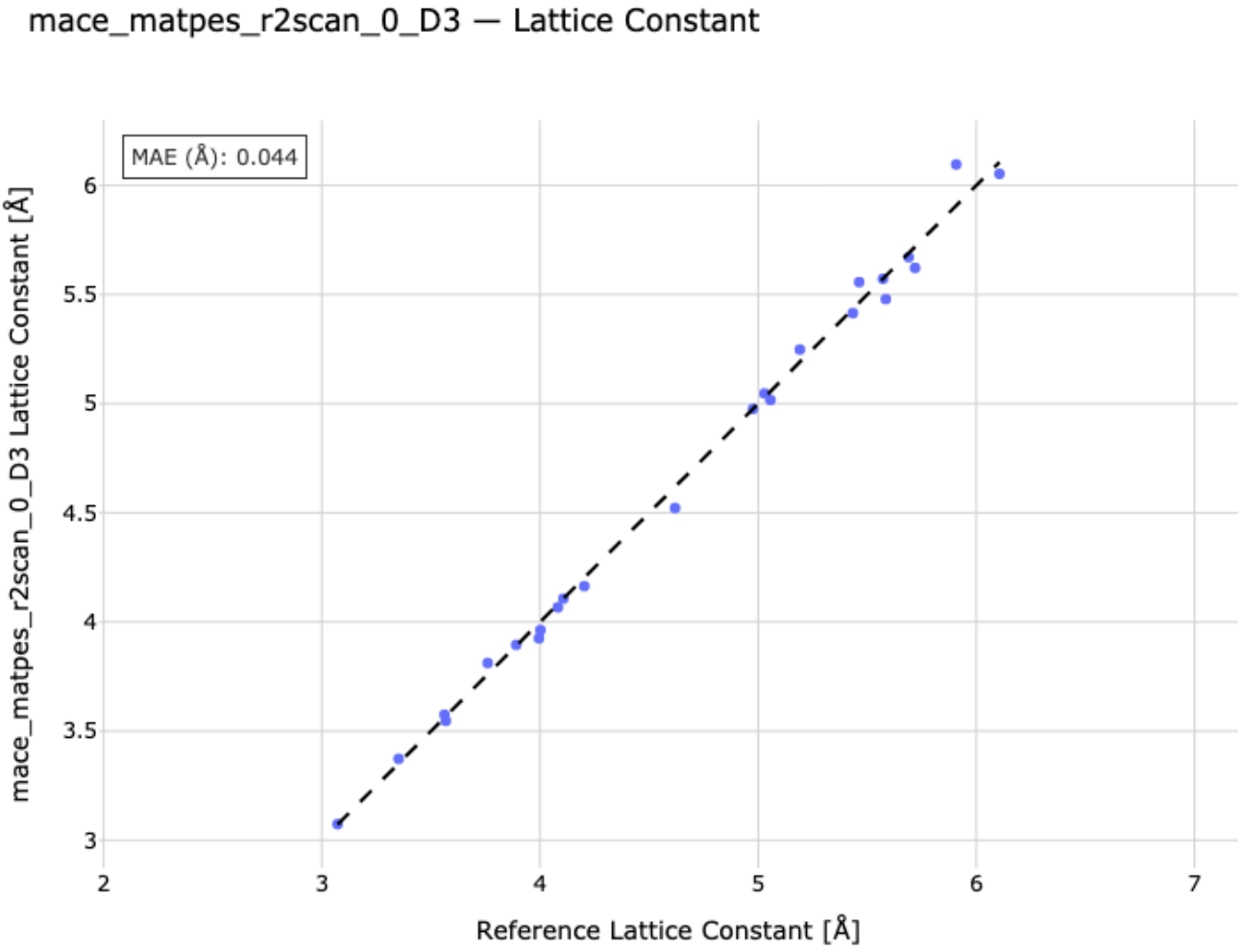
Element	DFT (Å)	mace_matpes_PBE_0_D3 (Å)	Δ	Δ/%
GaAs	5.69	5.704	0.014	0.25
Cu	3.568	3.556	-0.012	-0.34
C	3.562	3.533	-0.029	-0.81
LiCl	5.056	5.056	0	0
SiC(a)	3.072	3.069	-0.003	-0.1
SiC(c)	5.029	5.052	0.023	0.46



mace_matpes_r2scan_0_D3

Element	DFT (Å)	mace_matpes_r2scan_0_D3 (Å)	Δ	Δ/%
Ag	4.082	4.067	-0.015	-0.37
Pd	3.891	3.895	0.004	0.1
Rh	3.76	3.812	0.052	1.38
Li	3.352	3.373	0.021	0.63
Na	4.107	4.107	0	0
K	5.191	5.248	0.057	1.1
Rb	5.572	5.572	0	0
Cs	6.106	6.053	-0.053	-0.87

Element	DFT (Å)	mace_matpes_r2scan_0_D3 (Å)	Δ	Δ/%
Ca	5.463	5.557	0.094	1.72
Sr	5.908	6.096	0.188	3.18
Ba	4.976	4.976	0	0
Al	4.002	3.963	-0.039	-0.97
LiF	3.995	3.925	-0.07	-1.75
NaF	4.619	4.522	-0.097	-2.1
NaCl	5.585	5.479	-0.106	-1.9
MgO	4.203	4.164	-0.039	-0.93
Si	5.434	5.415	-0.019	-0.35
Ge	5.719	5.622	-0.097	-1.7
GaAs	5.69	5.671	-0.019	-0.33
Cu	3.568	3.547	-0.021	-0.59
C	3.562	3.575	0.013	0.36
LiCl	5.056	5.017	-0.039	-0.77
SiC(a)	3.072	3.074	0.002	0.07
SiC(c)	5.029	5.047	0.018	0.36



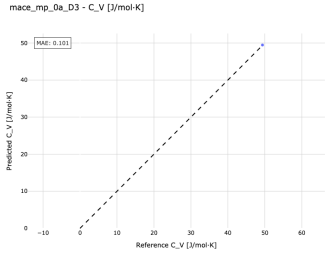
Phonon Dispersion Report

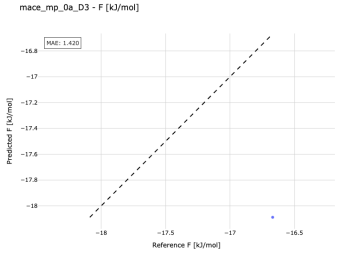
Phonon MAE Summary Table (300K)

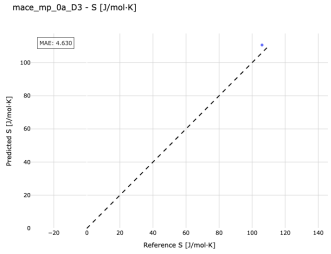
Model	ω_{max} [THz]	S [J/mol · K]	F [kJ/mol]	C_V [J/mol · K]	Phonon Score (avg)	Rank
mace_mp_0a_D3	0.631	4.63	1.42	0.101	1.696	6
mace_mp_0b3_D3	0.38	3.637	1.113	0.073	1.301	4
mace_mpa_0_D3	0.025	2.44	0.745	0.041	0.813	2
mace_omat_0_D3	0.002	2.116	0.646	0.037	0.7	1
mace_matpes_PBE_0_D3	0.476	3.658	1.12	0.075	1.332	5
mace_matpes_r2scan_0_D3	0.008	3.169	0.97	0.063	1.052	3

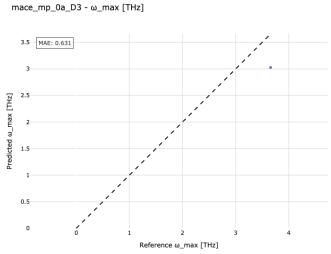
Scatter Plots

mace_mp_0a_D3









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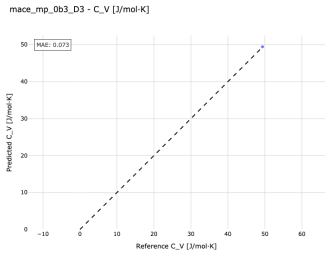

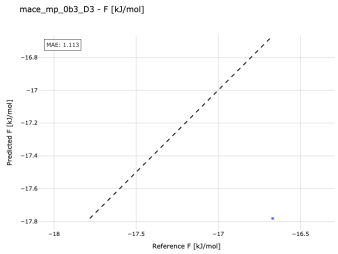

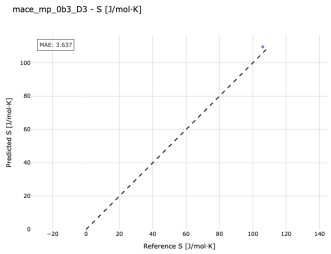

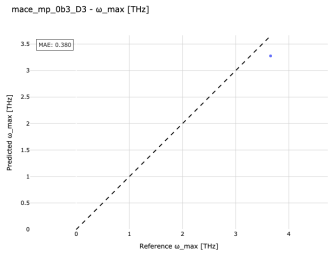

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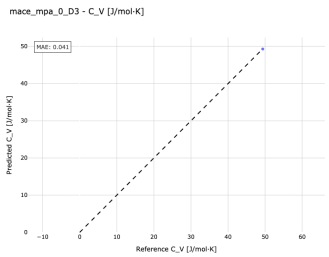

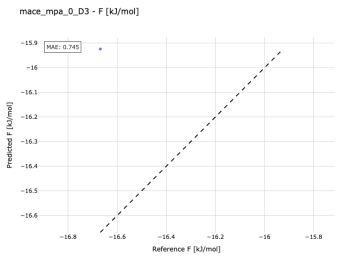

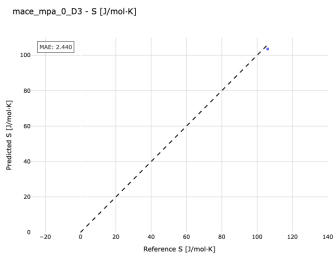

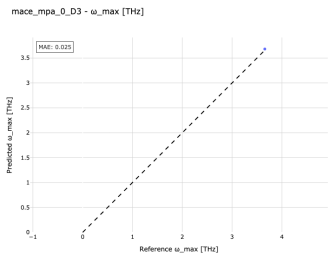

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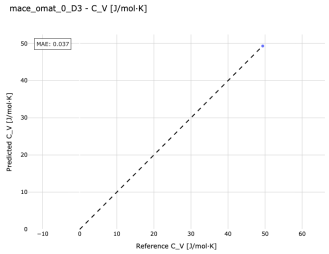

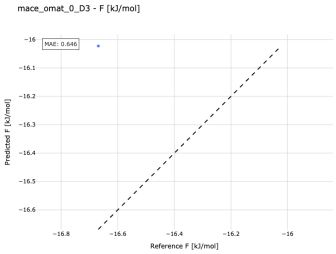

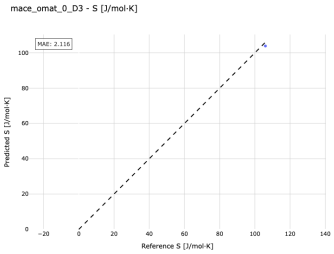

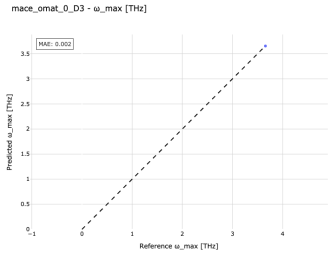

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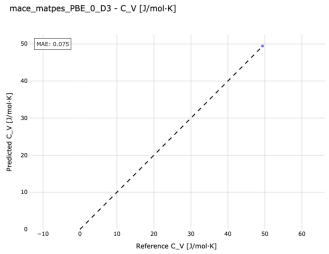

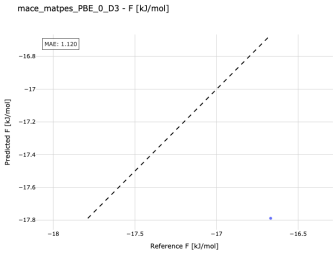

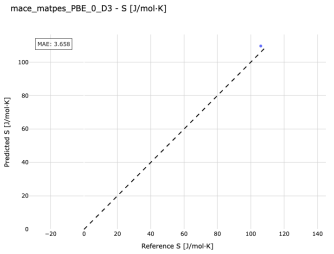

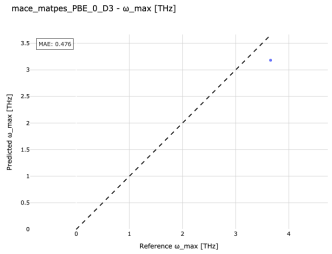

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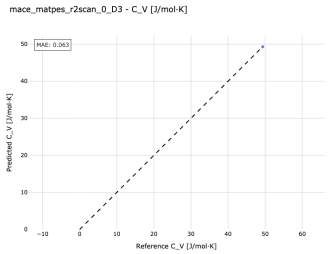

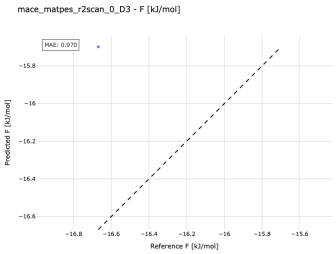

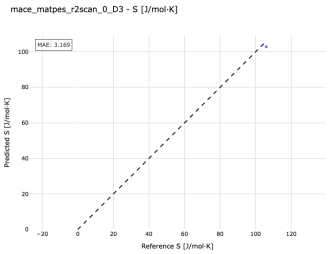

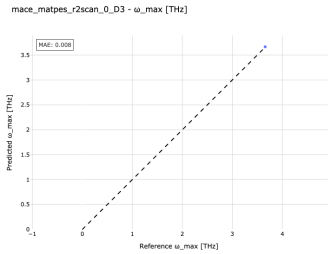

Dispersion Plots

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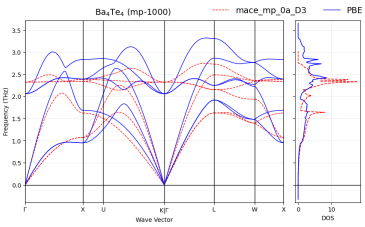

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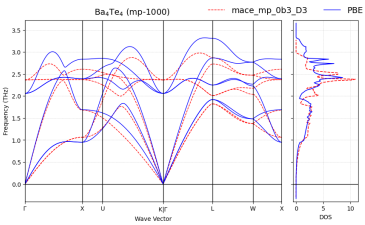

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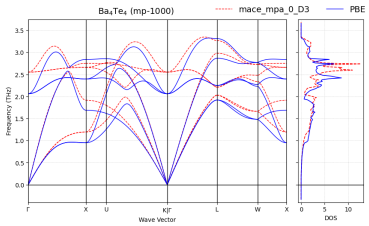

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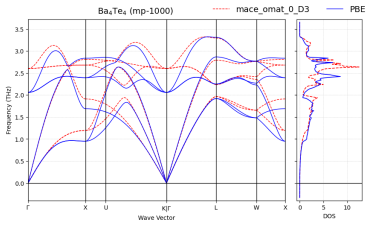

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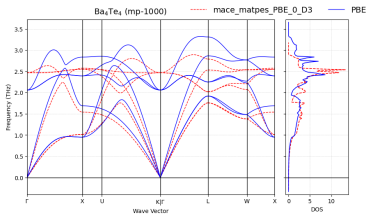
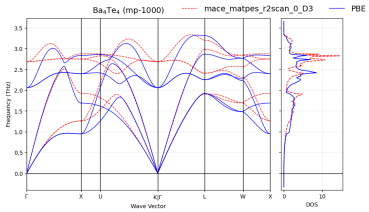
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