

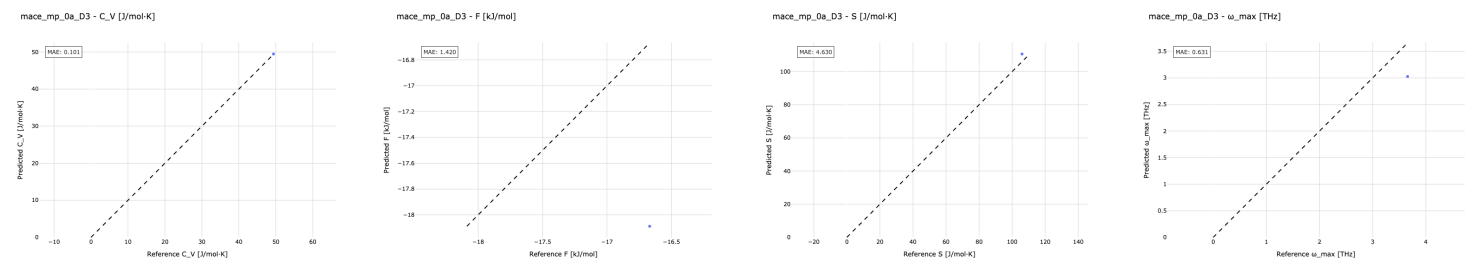
Phonon Dispersion Report

Phonon MAE Summary Table (300K)

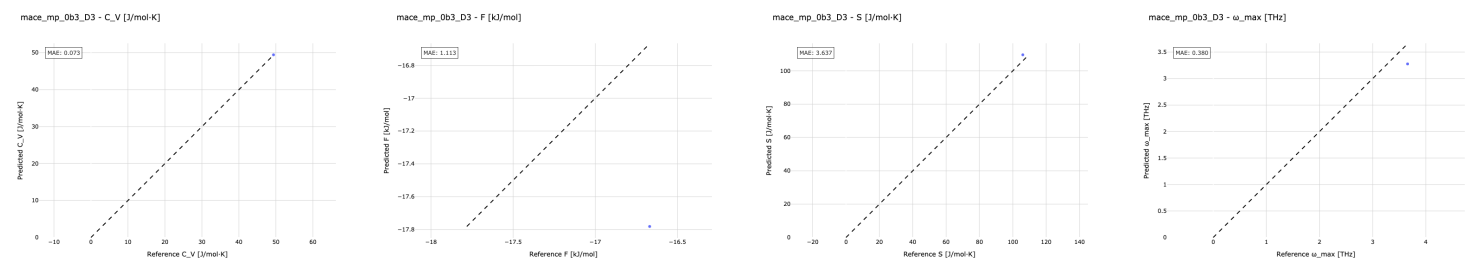
Model	ω_{max} [THz]	S [J/mol · K]	F [kJ/mol]	C_V [J/mol · K]	Phonon Score (avg)	Rank
mace_mp_0a_D3	0.631	4.63	1.42	0.101	1.696	6
mace_mp_0b3_D3	0.38	3.637	1.113	0.073	1.301	4
mace_mpa_0_D3	0.025	2.44	0.745	0.041	0.813	2
mace_omat_0_D3	0.002	2.116	0.646	0.037	0.7	1
mace_matpes_PBE_0_D3	0.476	3.658	1.12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

Scatter Plots

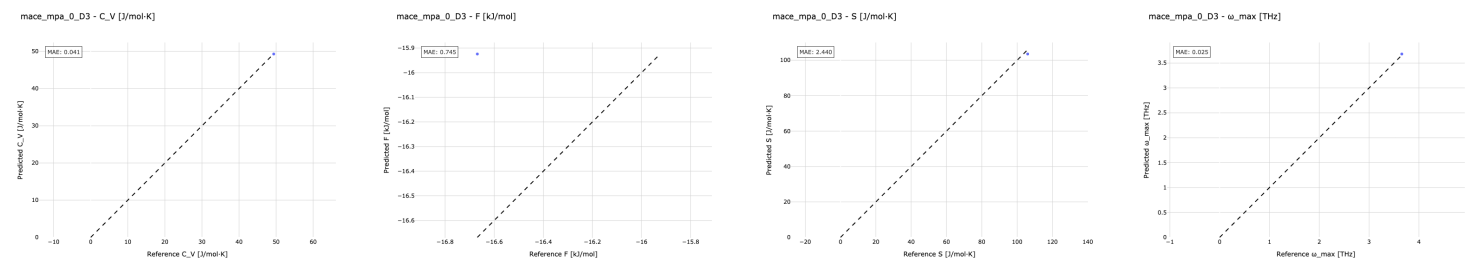
mace_mp_0a_D3



mace_mp_0b3_D3

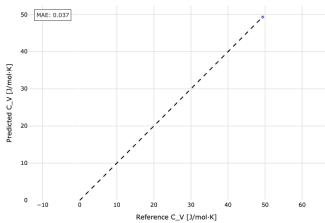


mace_mpa_0_D3

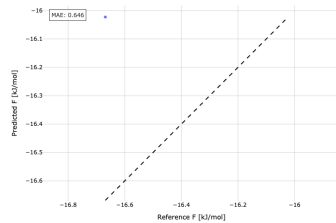


mace_omat_0_D3

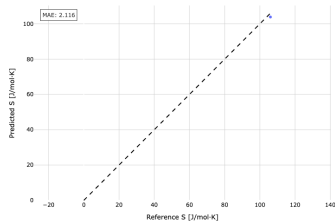
mace_omat_0_D3 - C_v [J/mol-K]



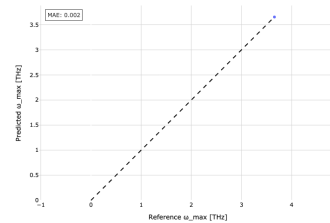
mace_omat_0_D3 - F [kJ/mol]



mace_omat_0_D3 - S [J/mol-K]

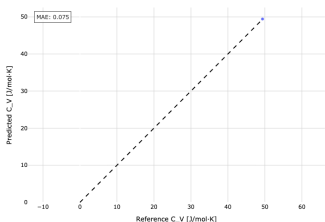


mace_omat_0_D3 - ω_{max} [THz]

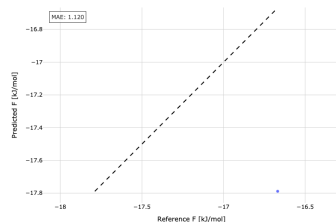


mace_matpes_PBE_0_D3

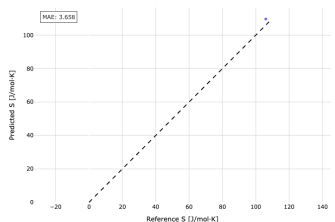
mace_matpes_PBE_0_D3 - C_v [J/mol-K]



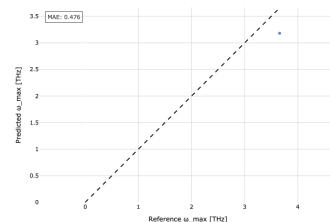
mace_matpes_PBE_0_D3 - F [kJ/mol]



mace_matpes_PBE_0_D3 - S [J/mol-K]

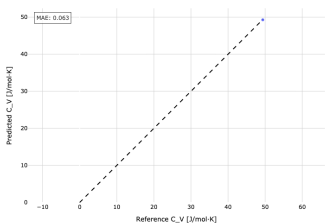


mace_matpes_PBE_0_D3 - ω_{max} [THz]

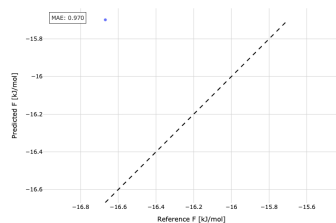


mace_matpes_r2scan_0_D3

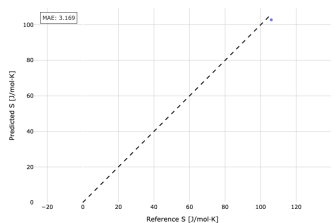
mace_matpes_r2scan_0_D3 - C_v [J/mol-K]



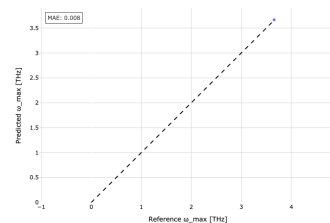
mace_matpes_r2scan_0_D3 - F [kJ/mol]



mace_matpes_r2scan_0_D3 - S [J/mol-K]

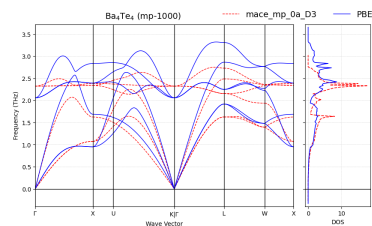


mace_matpes_r2scan_0_D3 - ω_{max} [THz]

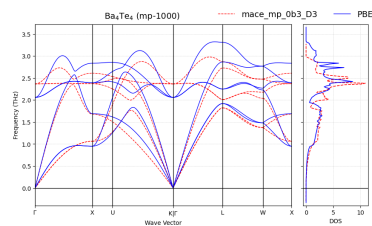


Dispersion Plots

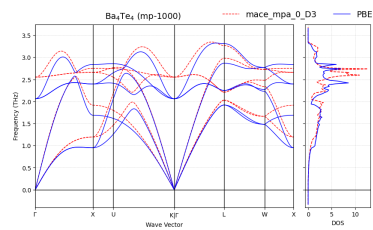
mace_mp_0a_D3



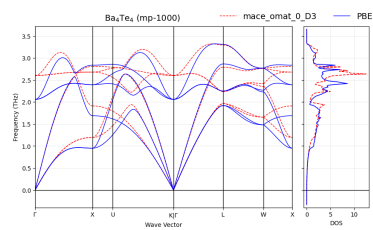
mace_mp_0b3_D3



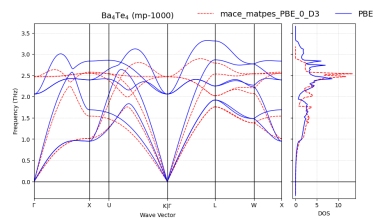
mace_mpa_0_D3



mace_omat_0_D3



mace_matpes_PBE_0_D3



mace_matpes_r2scan_0_D3

