

2B_PoSH_ph report

TIMING: 0.791 [ms/atom]

WEIGHT TABLE [E/F/V]

TiAl_phonons	5.00	200.000	1.0
TiAl_2000	100.00	5.000	1.0
Al_T1000	100.00	5.000	1.0
TiAl_dimer	5.00	0.500	1.0
Ti3Al_T2000	100.00	5.000	1.0
Al_dimer	5.00	0.500	1.0
default	20.00	1.000	1.0
Ti_dimer	5.00	0.500	1.0
TiAl3_T2000	100.00	5.000	1.0
Ti_T700	100.00	5.000	1.0
Ti_T1700	100.00	5.000	1.0
Ti_T1200	100.00	5.000	1.0

RMSE

config type	E [meV]		F [eV/A]		V [meV]	
Ti_T2700	5.74	0.000%	0.189	27.11%	27.6	3.41%
TiAl_phonons	1.70	0.000%	0.002	22.93%	13.9	23.26%
Al_T4000	7.12	0.007%	0.141	4.20%	26.6	1.46%
TiAl3_T5000	2.93	0.001%	0.261	5.48%	56.9	2.53%
TiAl_T5000	4.98	0.001%	0.302	7.19%	40.0	2.30%
Al_LD_1000K	7.22	0.007%	0.000	NaN%	81.6	11.16%
TiAl_2000	1.02	0.000%	0.068	6.72%	15.7	4.77%
Al_T1000	2.40	0.002%	0.035	4.64%	13.3	3.69%
Ti_hc..1000K	11.16	0.001%	0.117	29.35%	112.8	18.79%
TiAl_dimer	2.45	0.000%	0.160	0.10%	NaN	NaN%
Al_T2000	4.26	0.004%	0.084	4.92%	23.3	2.40%
Ti_bc..1000K	11.82	0.001%	0.103	17.79%	110.0	18.30%
Al_T3000	3.60	0.003%	0.122	4.38%	28.4	1.88%
Ti_T2200	2.87	0.000%	0.148	23.41%	25.7	2.81%
Ti3Al_T2000	0.83	0.000%	0.106	11.52%	21.4	4.00%
TiAl_T2000	1.16	0.000%	0.110	10.08%	18.1	2.92%
Ti_LD_1000K	10.24	0.001%	0.071	28.90%	36.9	4.62%

TiAl3..1000K	3.05	0.001%	0.052	7.12%	42.7	7.65%
Al_dimer	99.58	0.115%	0.576	1.08%	NaN	NaN%
Ti_dimer	6.77	0.000%	0.011	0.00%	NaN	NaN%
TiAl3_T2000	0.95	0.000%	0.090	4.16%	40.3	3.40%
Ti3Al..1000K	3.84	0.000%	0.059	9.09%	26.7	6.32%
Ti_T3700	5.29	0.000%	0.244	31.81%	37.2	4.76%
TiAl_..1000K	3.68	0.000%	0.028	3.74%	48.1	8.35%
Ti_T700	1.96	0.000%	0.092	26.18%	31.9	2.64%
Ti_T3200	5.54	0.000%	0.222	30.29%	30.7	3.64%
Ti_T1700	2.61	0.000%	0.133	23.79%	20.6	1.97%
Ti3Al_T5000	5.19	0.000%	0.320	12.12%	42.5	4.37%
Ti_T1200	1.71	0.000%	0.111	24.93%	21.5	1.91%
Ti_T4200	8.46	0.001%	0.260	32.42%	36.7	5.45%
TiAl_5000	5.13	0.001%	0.288	7.17%	42.4	2.75%
set	8.05	0.001%	0.190	6.73%	79.7	11.35%

