

PoSH report

RMSE

config type	E [meV]		F [eV/Å]		V [meV]	
Ti_T2700	5.17	0.000%	0.215	30.82%	42.2	5.22%
Al_T4000	6.28	0.006%	0.159	4.74%	30.0	1.64%
TiAl3_T5000	3.40	0.001%	0.281	5.89%	57.9	2.58%
TiAl_T5000	3.62	0.000%	0.326	7.77%	42.6	2.45%
TiAl_dimer2	320.66	0.038%	0.356	98.82%	NaN	NaN%
Al_T1000	3.50	0.003%	0.042	5.54%	15.6	4.34%
TiAl_2000	0.50	0.000%	0.083	8.19%	16.4	5.00%
TiAl_dimer	1736.75	0.206%	6.604	13.87%	NaN	NaN%
Al_T2000	6.70	0.006%	0.094	5.50%	25.4	2.61%
Al_dimer2	300.00	0.283%	0.284	104.41%	NaN	NaN%
Al_T3000	4.40	0.004%	0.136	4.91%	34.0	2.25%
Ti_T2200	3.30	0.000%	0.176	27.75%	30.4	3.33%
Ti3Al_T2000	1.55	0.000%	0.138	15.02%	23.0	4.31%
TiAl_T2000	1.63	0.000%	0.119	10.83%	18.8	3.03%
Al_dimer	1432.33	1.393%	6.223	30.62%	NaN	NaN%
Ti_dimer2	314.30	0.020%	0.731	142.39%	NaN	NaN%
Ti_dimer	3476.51	0.219%	9.896	13.07%	NaN	NaN%
TiAl3_T2000	1.93	0.000%	0.141	6.53%	42.2	3.56%
Ti_T3700	5.07	0.000%	0.271	35.35%	47.5	6.08%
Ti_T700	4.76	0.000%	0.118	33.59%	65.7	5.43%
Ti_T3200	6.09	0.000%	0.246	33.55%	37.4	4.43%
Ti_T1700	4.26	0.000%	0.163	29.22%	26.8	2.57%
Ti3Al_T5000	5.13	0.000%	0.359	13.60%	48.7	5.01%
Ti_T1200	2.37	0.000%	0.139	31.16%	24.4	2.17%
Ti_T4200	8.74	0.001%	0.289	35.98%	44.2	6.56%
TiAl_5000	2.98	0.000%	0.316	7.86%	46.0	2.99%
set	665.50	0.061%	0.456	12.55%	39.4	3.18%

vcat(energy_2b_11, energy_2b_12, energy_2b_22) = [22.4695, 19.3535, 16.7083, 14.4551, 12.5298, 10.8801, 9.46306, 8.24294, 7.16619, 6.18465, 5.30131, 4.51526, 3.8224, 3.21664, 2.69078, 2.23717, 1.84809, 1.51612, 1.23426, 0.996094, 0.795777, 0.628083, 0.488376, 0.372578, 0.277123, 0.198911, 0.135266, 0.0838789, 0.0427731, 0.0102577, -0.0151078, -0.0345471, -0.0490966, -0.059

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