

Supplementary Material

In the supplementary materials, we provide the learning curves for active learning using MTP and DeePMD (see Section 0.1), the absolute differences in elastic constants predicted by MTP and DeePMD relative to DFT for both Comparison 1 and Comparison 2 (see Section 0.2), and RDF comparisons for cases not presented in the main text (see Section 0.3).

0.1 Active learning curves

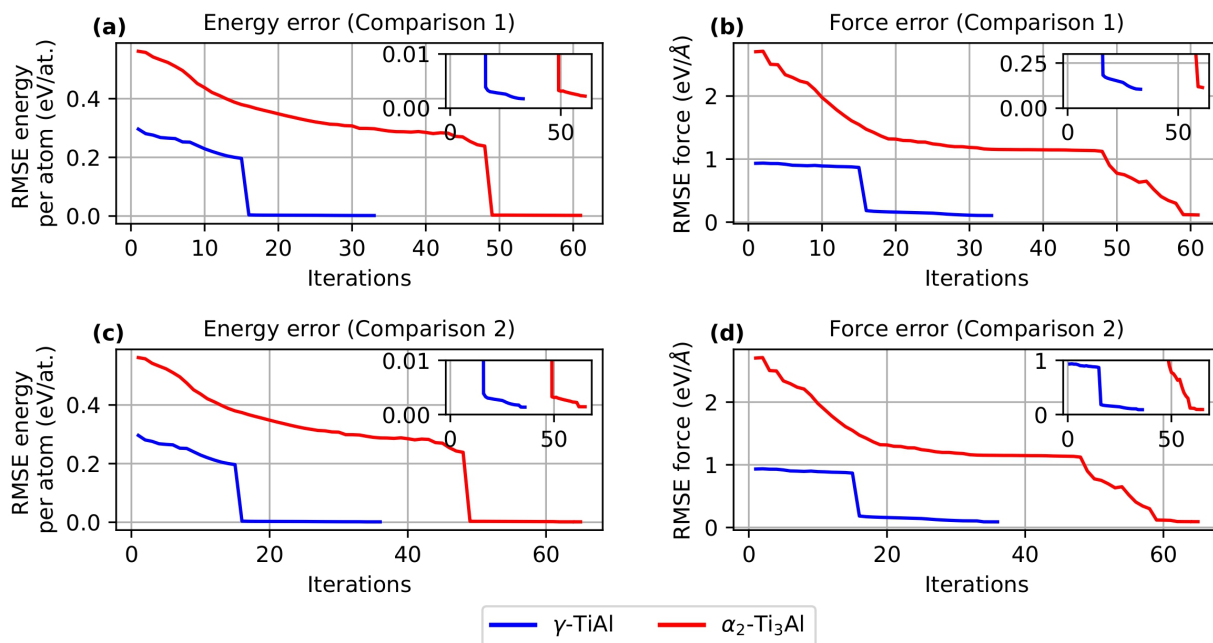


Figure S1. Learning curves for MTP showing the RMSE in energy per atom and force for γ -TiAl and α_2 -Ti₃Al. The RMSE values are plotted as a function of the active learning iterations. Panels (a) and (b) correspond to Comparison 1, where both active and passive learning potentials were trained using the same number of samples, while panels (c) and (d) correspond to Comparison 2, where the training dataset sizes were varied to achieve comparable error levels.

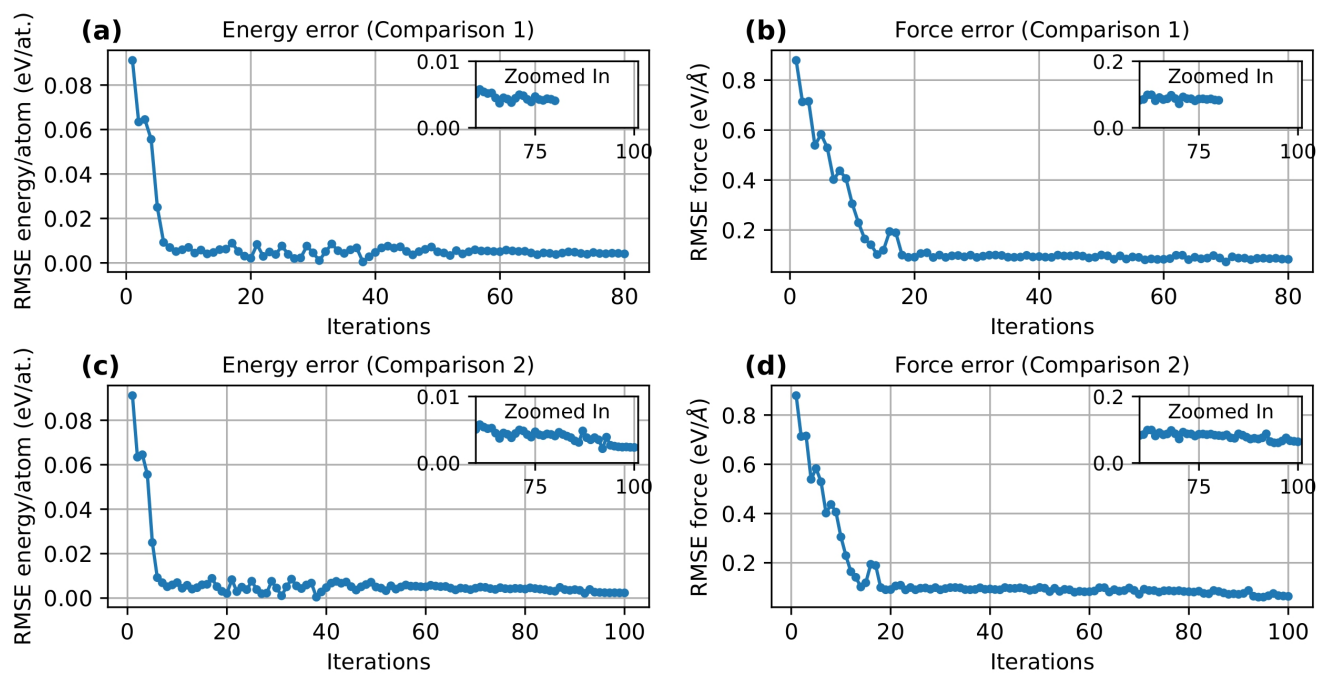


Figure S2. Learning curves for DeePMD showing the RMSE in energy per atom and force. The RMSE values are plotted as a function of the active learning iterations. Panels (a) and (b) correspond to Comparison 1, where both active and passive learning potentials were trained using the same number of samples, while panels (c) and (d) correspond to Comparison 2, where the training dataset sizes were varied to achieve comparable error levels.

Table S1. Comparison of RMSE values of energy/atom and force for MTP (using Dataset-B for γ -TiAl and Dataset-D for α_2 -Ti₃Al) and DeePMD (using Dataset-F).

Potential	Energy/atom (eV/atom)	Force (eV/Å)
MTP (γ -TiAl / α_2 -Ti ₃ Al)	1.32×10^{-3} / 1.23×10^{-3}	80.14×10^{-3} / 94.44×10^{-3}
DeePMD	1.07×10^{-3}	93.14×10^{-3}

0.2 Absolute difference of elastic constants.

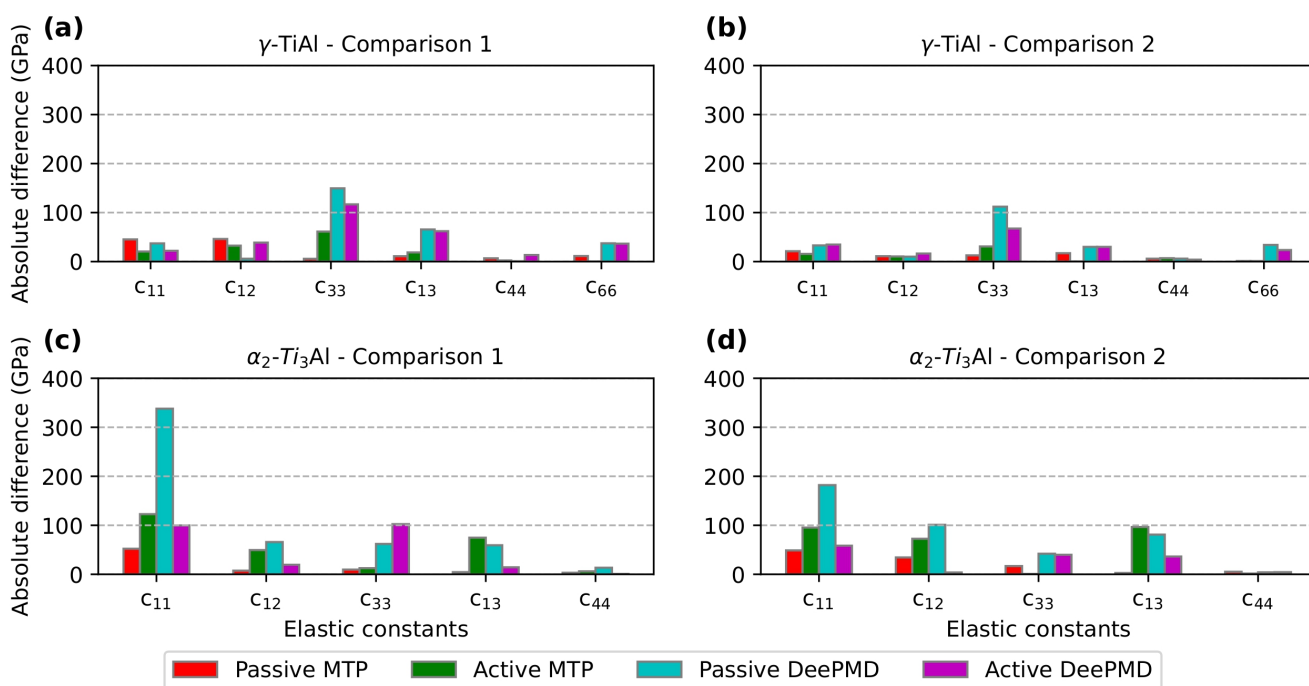


Figure S3. Absolute differences in elastic constants relative to DFT for active and passive learning potentials developed using MTP and DeePMD. Panels (a) and (b) correspond to γ -TiAl, while panels (c) and (d) correspond to α_2 -Ti₃Al. For Comparison 1, both potentials were trained using the same number of samples to enable a direct performance evaluation, whereas in Comparison 2 the training dataset sizes were varied to achieve comparable error levels. Note the unit of elastic constant is Gigapascal (GPa) and they are computed at 300 K.

0.3 Radial distribution function

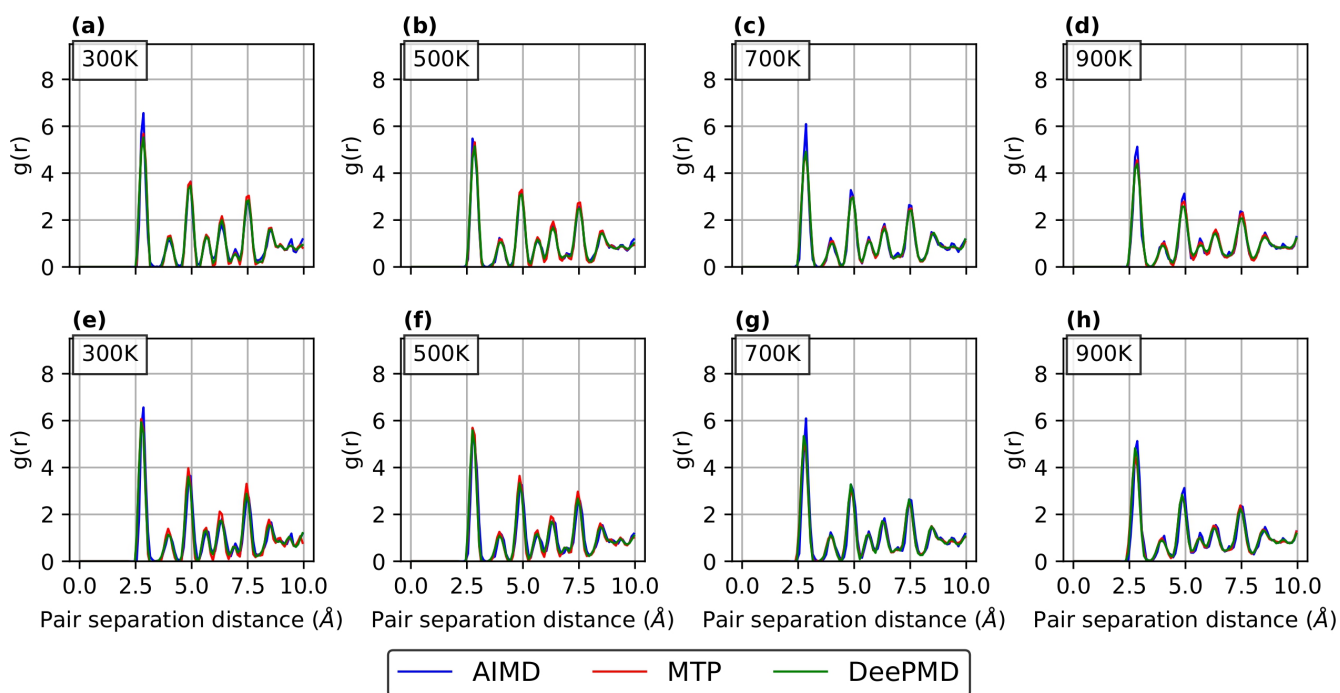


Figure S4. RDF curves for γ -TiAl with a 5.6 at% Nb configuration obtained from passive and active learning potentials, compared with AIMD results at 300 K, 500 K, 700 K, and 900 K for both MTP and DeePMD. The top row (panels a–d) displays the AIMD and active learning potential results, while the bottom row (panels e–h) shows the curves from the passive learning potential. These results correspond to Comparison 2, where the training dataset sizes were adjusted to achieve comparable error levels.

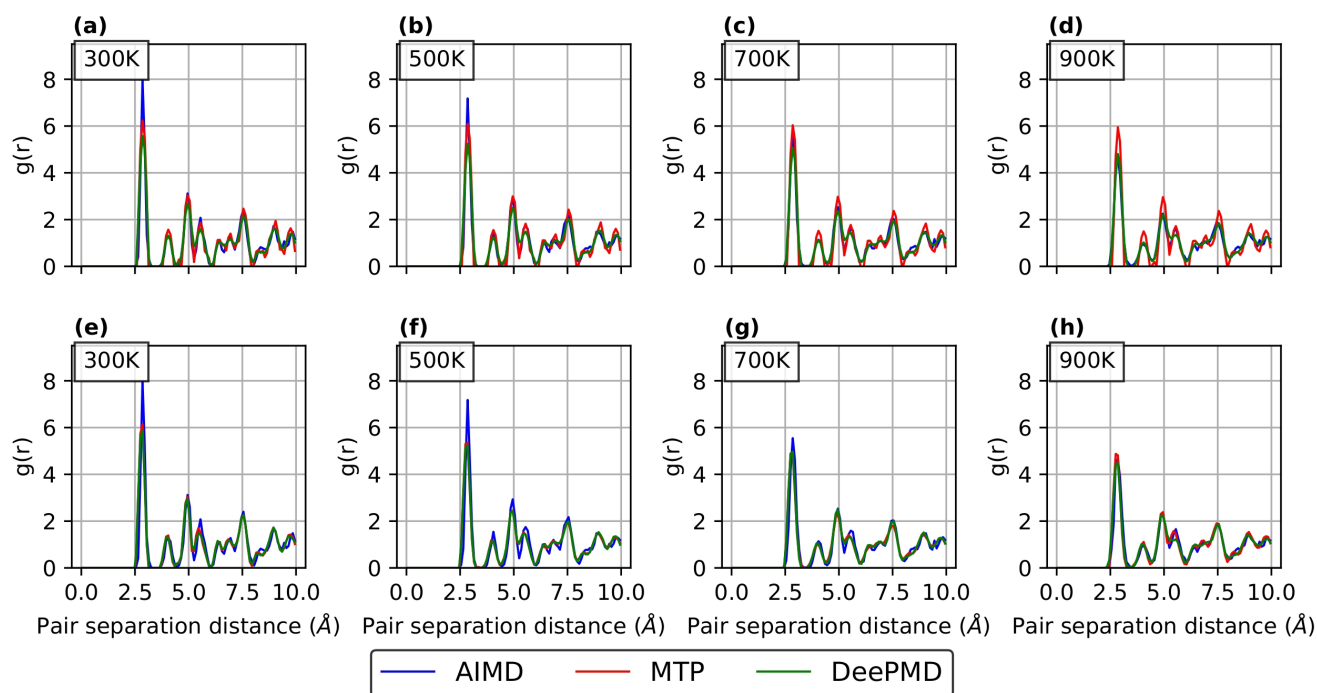


Figure S5. RDF curves for α_2 -Ti₃Al with a 2.3 at% Nb configuration obtained from passive and active learning potentials, compared with AIMD results at 300 K, 500 K, 700 K, and 900 K for both MTP and DeePMD. The top row (panels a–d) displays the AIMD and active learning potential results, while the bottom row (panels e–h) shows the curves from the passive learning potential. These results correspond to Comparison 2, where the training dataset sizes were adjusted to achieve comparable error levels.