Supplementary Materials for

"Hydrogen Diffusion in Magnesium Using Machine Learning Potentials"

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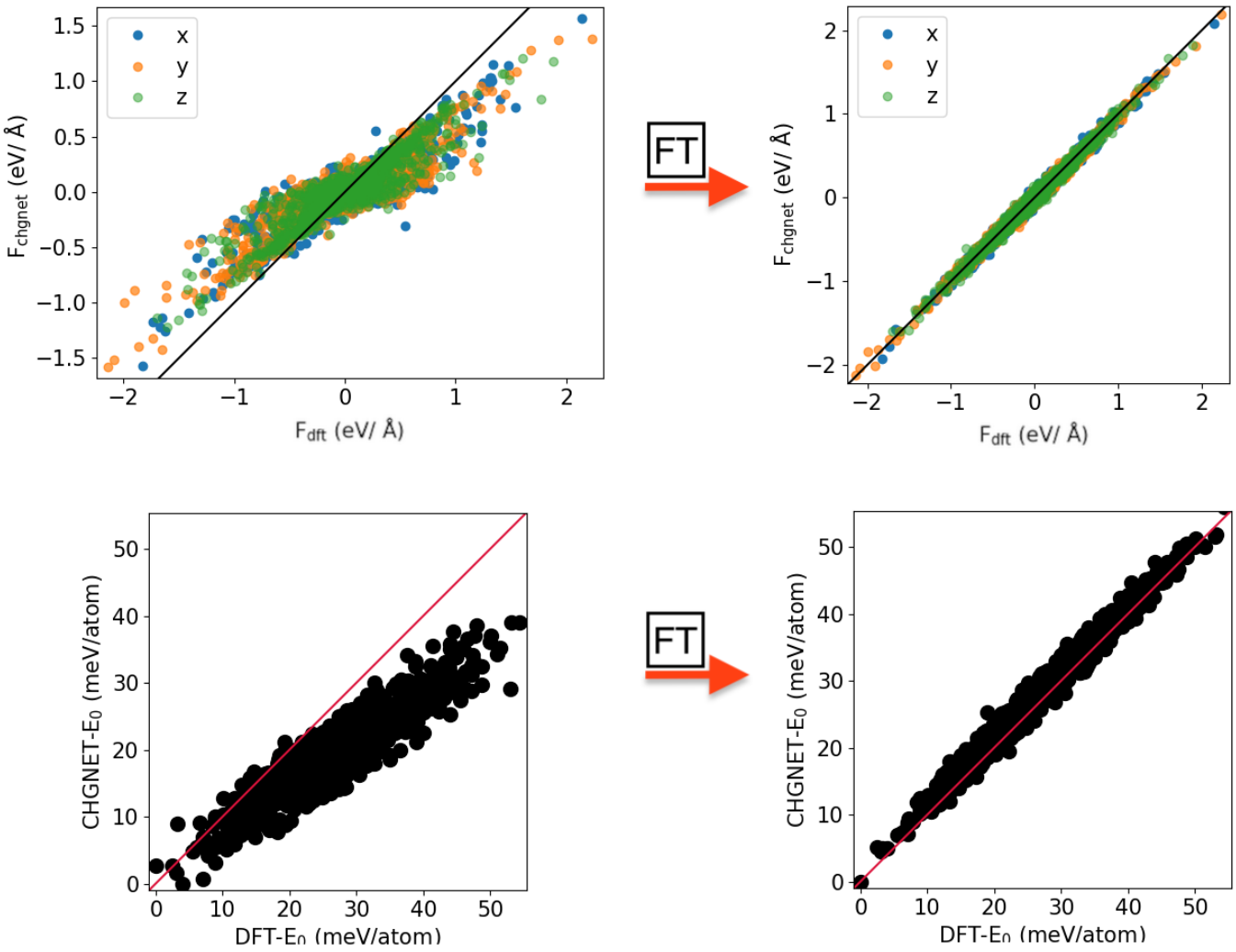
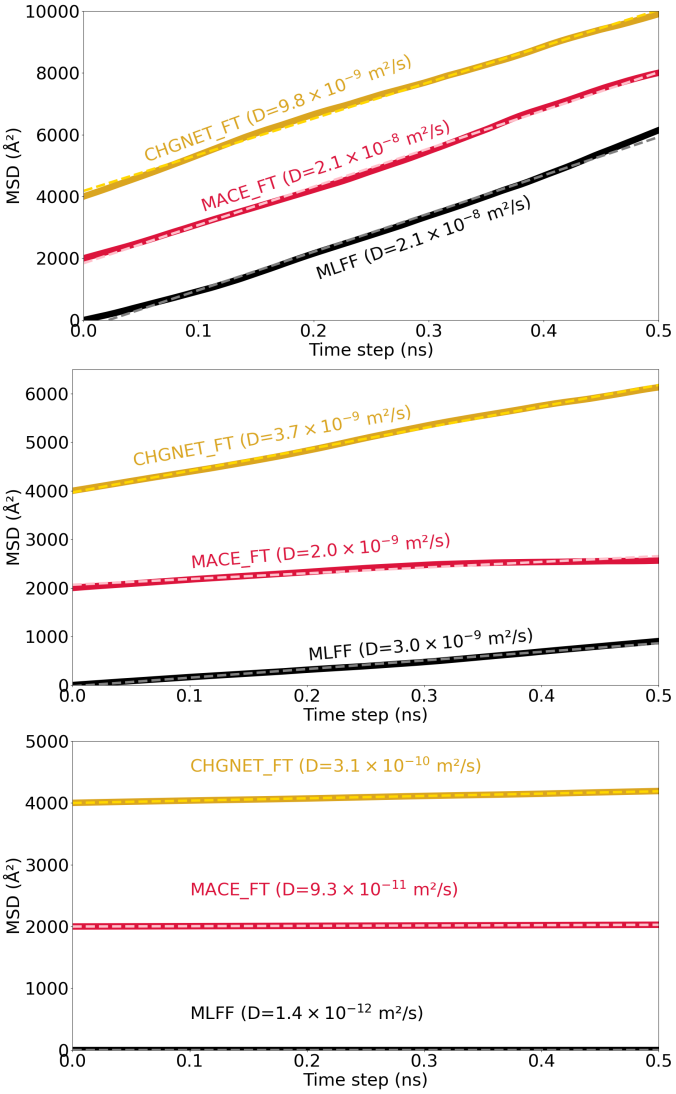
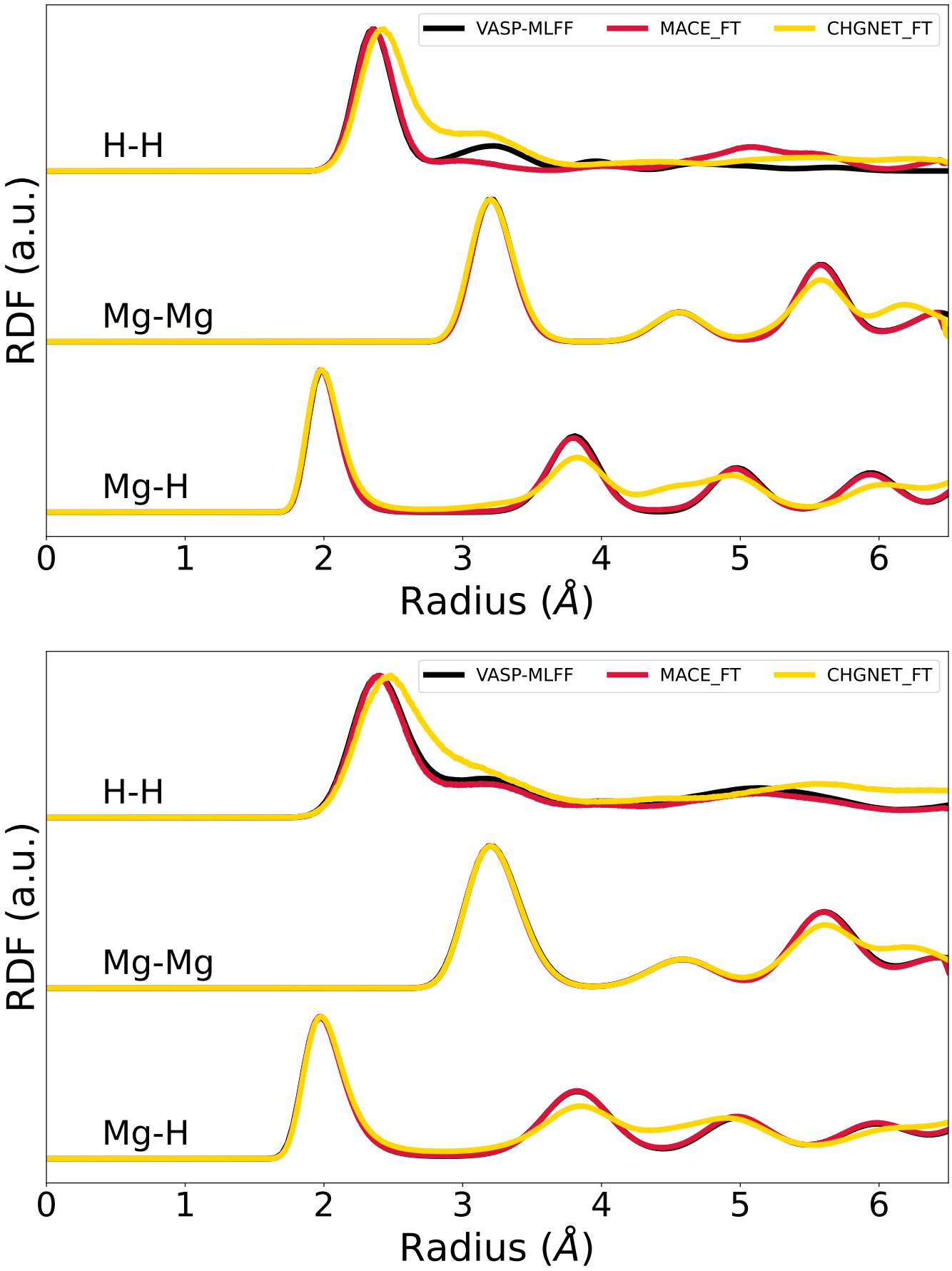


Supplementary Figure 1: Comparison between the pre-trained (CHGNET_MP) and fine-tuned (FT) performances of CHGNet in a validation over 1000 DFT configurations extracted during the diffusion simulations, evaluated as a parity plot between DFT energies and forces and the corresponding predictions. We report the relevant RMSE values in the main text.



Supplementary Figure 2: Linear region of the Mean Square Displacement for the VASP-MLFF, CHGNET_FT and MACE_FT at three different average constant temperatures of 673K (top), 480K (center) and 300K (bottom).



Supplementary Figure 3: Radial distribution function at different temperatures for the best performing models, at 300 K on top and 480K at the bottom.