Supplementary Information

Machine Learning Potential for Modelling H_2 Adsorption/Diffusion in MOFs with Open Metal Sites

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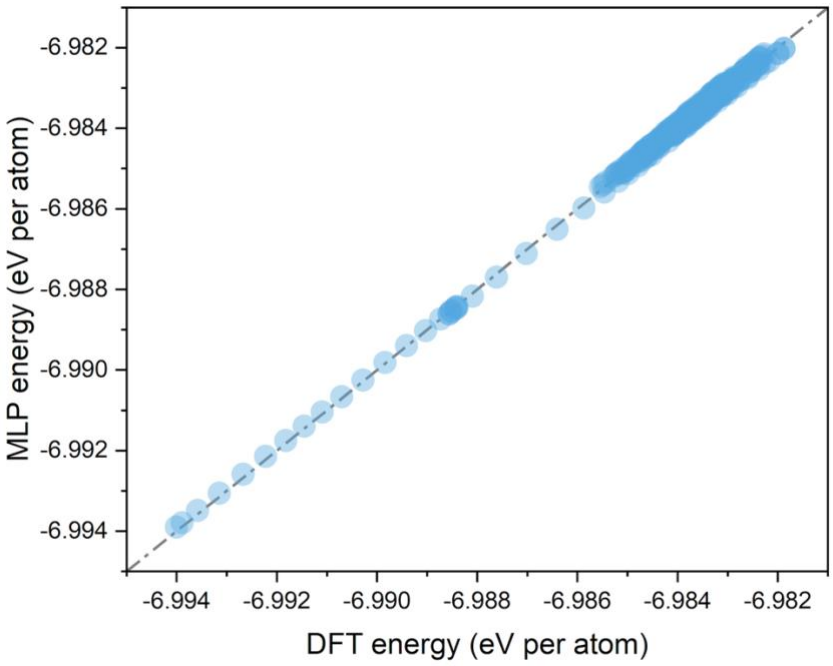
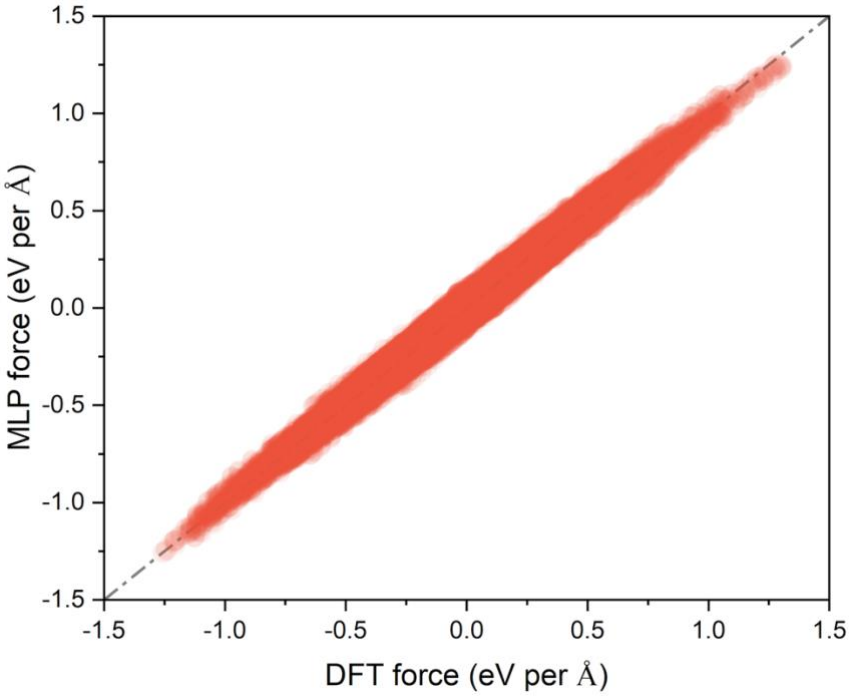
Supplementary Table S1 | Data preparation for the MLP training of the H_2@Al-soc-MOF-1d system (including DFT-optimizations and AIMD runs at 10-100K).

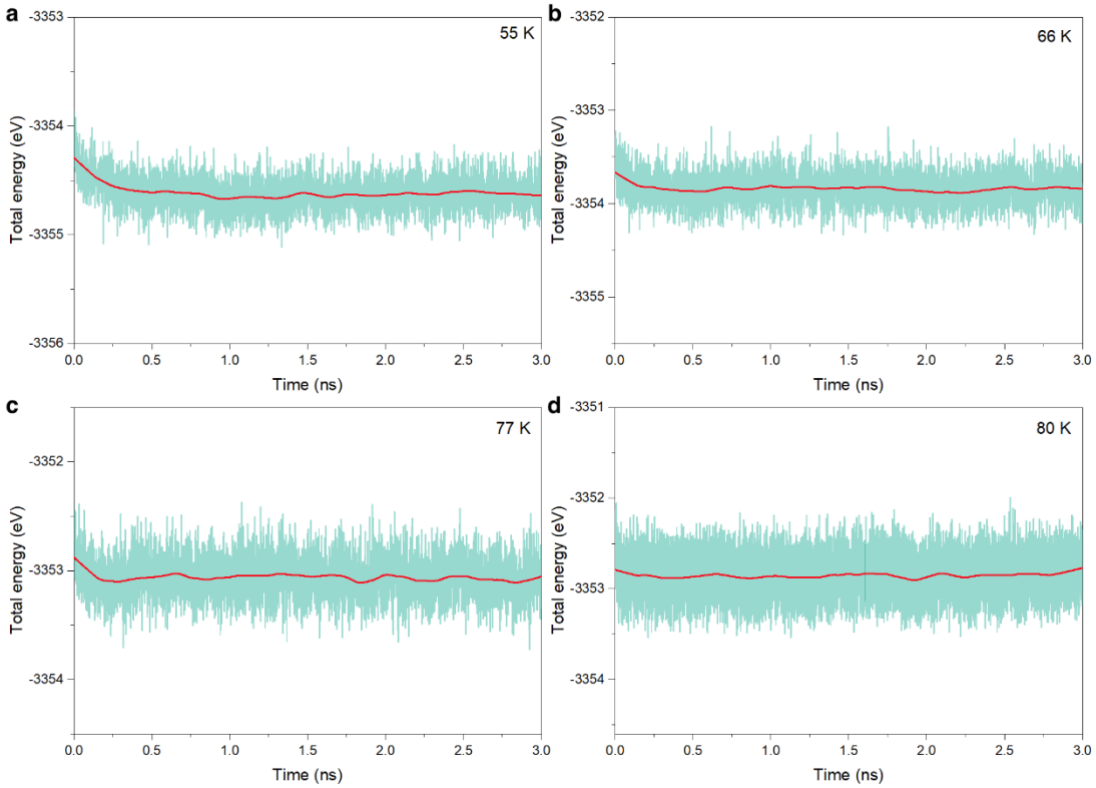
H_2 loading [per unit-cell]	**Number of atoms**	**Number of configurations**
8	448	1575
24	480	11574
40	512	2236
57	546	2148
103	638	2204
134	700	1882



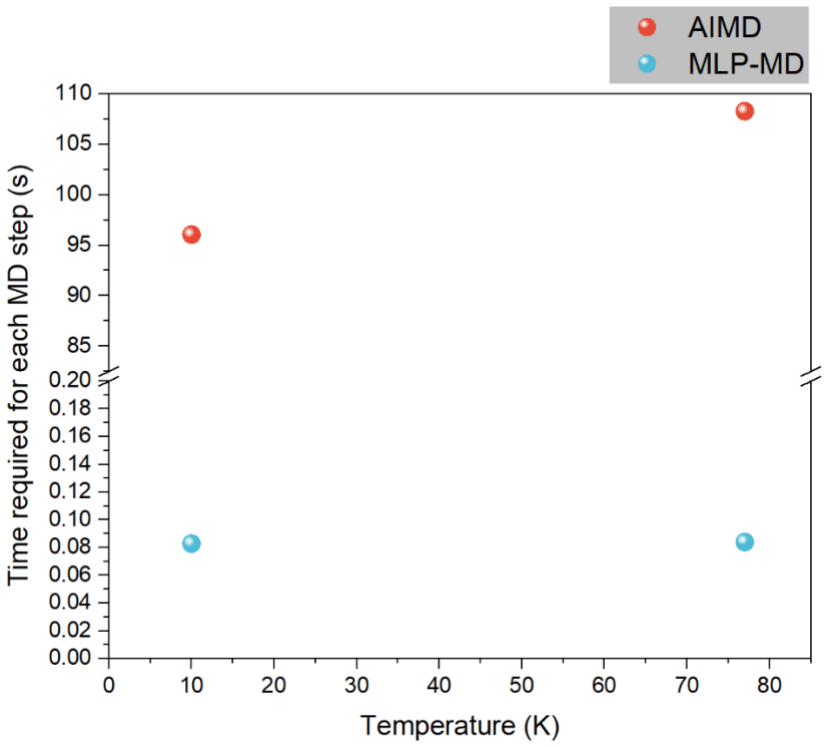
Supplementary Fig. S1 | MLP derived energies *vs* the corresponding DFT values in the validation dataset.



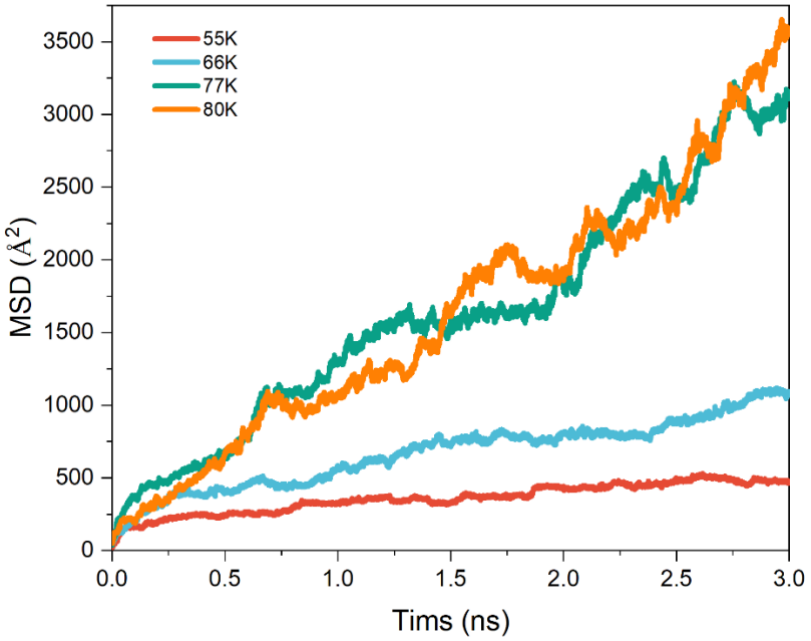
Supplementary Fig. S2 | MLP derived forces *vs* the corresponding DFT values in the validation dataset.



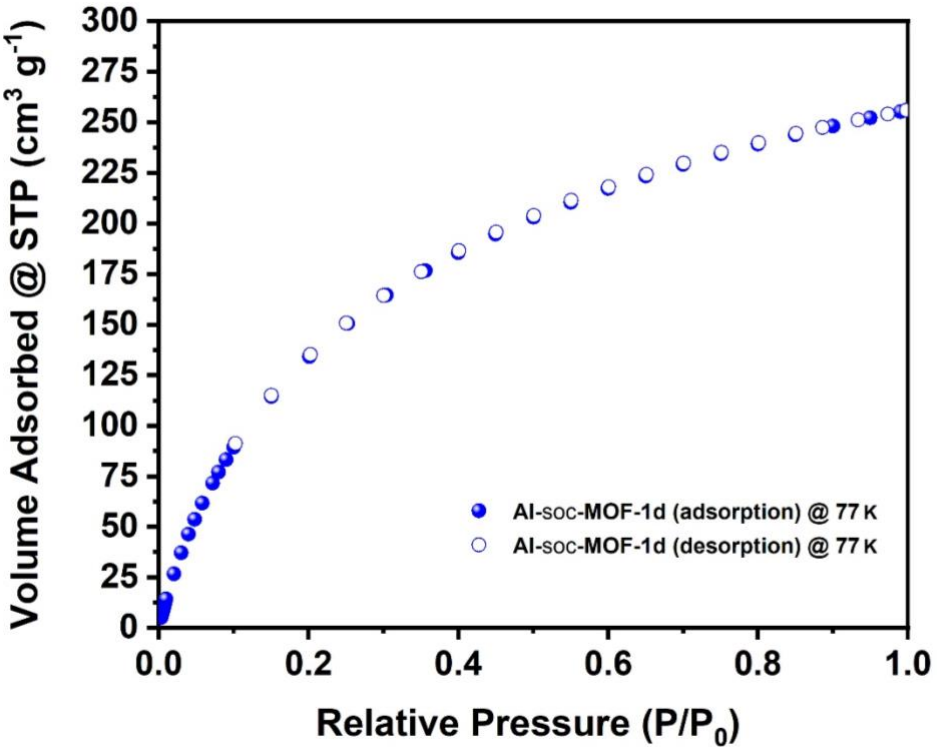
Supplementary Fig. S3 | Evolution of the energy over the MLP-MD trajectories for 24 H_2@Al-soc-MOF at (a-d) 55 K, 66 K, 77 K, and 80 K, respectively.



Supplementary Fig. S4 | The CPU time comparison between AIMD and MLP-MD simulations at 10K and 77K temperatures (24 H_2 loading per unit-cell). For each system, the same CPU (192-cores) was used to compute the average time per MD time step in seconds.



Supplementary Fig. S5 | MLP-MD simulated mean square displacement (MSD) of H_2 molecules (24 H_2 per unit-cell loading) *versus* simulation time at different temperatures.



Supplementary Fig. S6 | Experimental H_2 adsorption isotherms collected at 77 K up to 1 bar.