Supplementary information: Online Test-time Adaptation for Interatomic Potentials

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Hyperparameters

We show the detailed hyperparameters for different datasets in Table S1, Table S2, and Table S3. We employ the learning rate adjustment strategy as [1]. Initially, we warm up the learning rate, followed by utilizing StepLR learning rate strategies during training. Specifically, the learning rate is reduced by a decay ratio at every fixed epoch, which we refer to as the step size. For all experiments, some hyperparameters are set to fixed values without optimization, while others are optimized through grid search.

Table S1 Search space for hyperparameters on MD17.

Hyperparameters	Search space
Number of interaction blocks (SchNet)	6
Number of interaction blocks (PaiNN)	3,4
Cutoff distance	5.0, 6.0, 10.0
Batch size	1, 2, 4, 16, 32
Initial learning rate	1e-3, 5e-4, 1e-4
Learning rate strategy	StepLR
Learning rate decay ratio	0.4, 0.5, 0.6
Learning rate step size	50, 100, 200
Learning rate warmup factor	0.7
Max # of Epochs	500, 1000, 2000

Table S2 Search space for hyperparameters on ISO17.

Hyperparameters	Search space
Number of interaction blocks (SchNet)	5,6
Number of interaction blocks (PaiNN)	3,4
Cutoff distance	5.0, 6.0
Batch size	32, 64, 128
Initial learning rate	1e-3, 1e-4, 5e-5
Minimum learning rate	1e-7
Learning rate cosine decay ratio	0.0, 0.1, 0.2
Learning rate step size	50, 100, 200
Learning rate warmup factor	0.7
Max # of Epochs	50

Table S3 Search space for hyperparameters on Electrolyte/Liquid water.

Hyperparameters	Search space
Number of interaction blocks (SchNet)	5, 6
Number of interaction blocks (PaiNN)	3, 4, 5
Batch size	1, 2, 4, 8
Initial learning rate	1e-3, 5e-4, 1e-3
Learning rate strategy	StepLR
Learning rate decay ratio	0.4, 0.5, 0.6
Learning rate step size	50, 100, 200
Learning rate warmup factor	0.7
Max # of Epochs	500, 1000, 2000

Additional Results

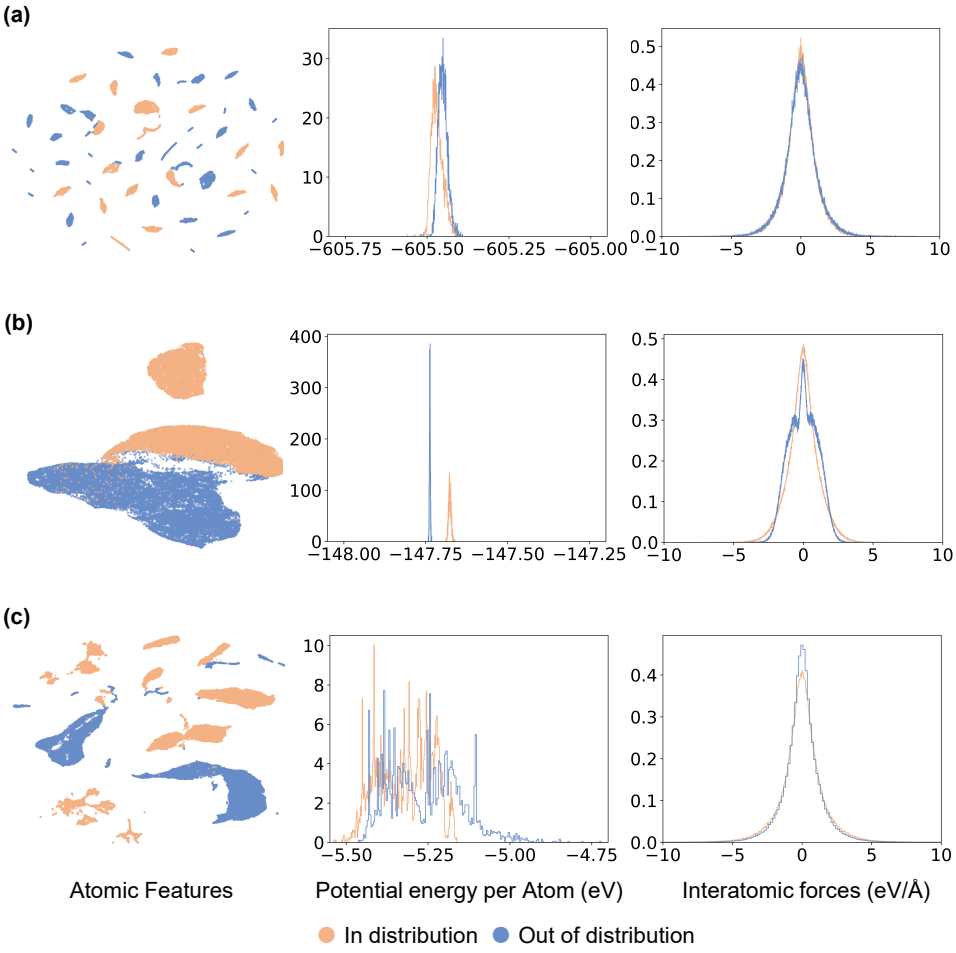

Fig. S1 Distribution shift characterization. (a) ISO17. (b) Water. (c) Electrolyte solutions. Left: feature visualization. The representation of atomic features is generated by UMAP dimension reduction method on SOAP descriptors. Middle: distribution of potential energy. Right: distribution of force.

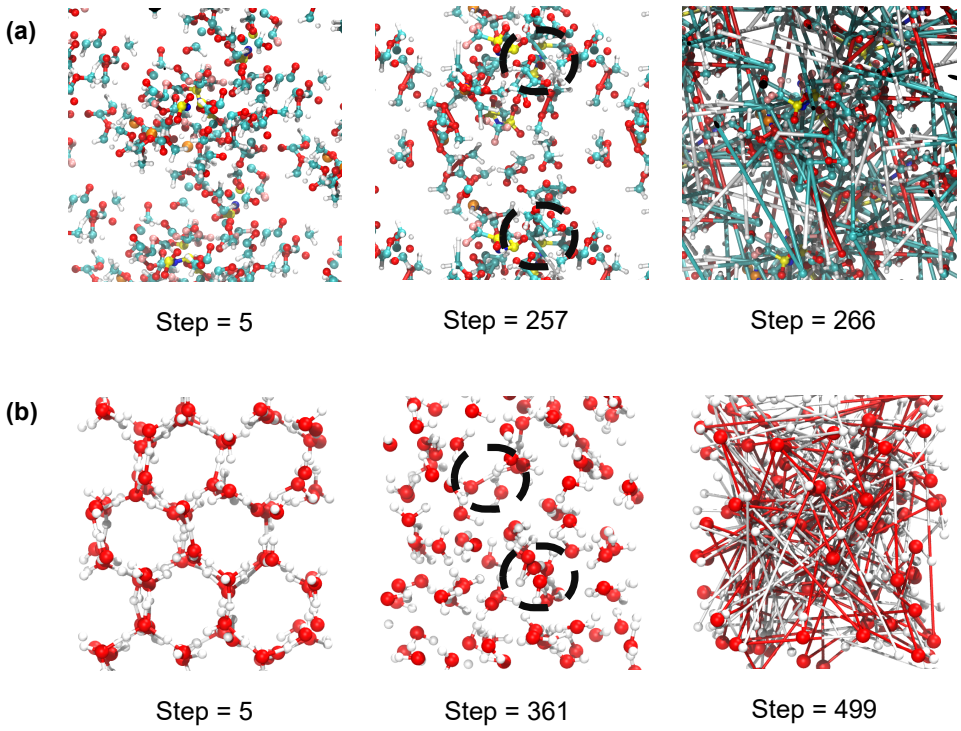

Fig. S2 Trajectories of Electrolyte solution and Water. The Snapshots of the MD trajectories of (a) electrolyte solution (1M $[Na^+][Tf_2N^-]$ in EC + DMC) and (b) ice using the baseline PaiNN model at 300K. Occurrences of unrealistic molecular configurations (circled by black dashed lines) will cause a collapse during MD simulations using MLIPs.

Table S4 Ablation study on liquid water dataset. Energy and Force MAEs are reported in unit of [eV] and [eV/Å], respectively. T1 indicates the noise intensity prediction task, T2 indicates the atomic feature recover task, T3 indicates the pseudo force recover task, and TAIP indicates all the 3 tasks are involved.

	PaiNN	PaiNN-T1	PaiNN-T2	PaiNN-T1+T2	PaiNN-T2+T3	PaiNN-TAIP
Energy	1.193	0.574	0.871	0.563	0.549	**0.423**
Force	0.083	0.065	0.078	0.062	0.060	**0.055**

References

[1] Liu, Y., Wang, L., Liu, M., Lin, Y., Zhang, X., Oztekin, B., Ji, S.: Spherical message passing for 3d molecular graphs. In: International Conference on Learning Representations (ICLR) (2022)