S1. Construction of machine learning potential

S1.1. *Ab initio* MD simulations

The VASP code [1–3] is used with potpaw-PBE.54 [4] pseudopotentials to perform *ab initio* molecular dynamic (AIMD) simulations to collect the energies, atomic force, and stress as datasets for the training of the machine learning based neuroevolution potential (NEP). The system of water for AIMD calculations contains 180 molecules with 360 atoms. The cutoff energy of 400 eV is used. A 3×3×3 Γ-centered grid of k points in the irreducible Brillouin zone is used. To fully consider the effect of temperature on phase transition, AIMD is performed in the isothermal-isobaric (NPT) ensemble at the temperatures of 50 K, 100 K, 300 K, 500 K, 600 K, 700 K and 1000 K. The time step is 0.25 fs. The 12000 and 5000 AIMD atomic configurations and the corresponding atomic forces, total energies, and stresses are used to train and test NEP potential, respectively.

S1.2. Machine learning potential

We employ a NEP potential developed by Fan et al. [5] as a machine learning potential model to describe the complex interactions between and inside the water molecules. With the trained NEP, we would be able to do further lattice dynamic and molecular dynamic calculations by using the GPUMD software [6]. To begin with, the trained NEP is tested by comparing the energies and atomic forces predicted by DFT and NEP predictions, which reveals a good agreement between the two calculations (See Fig. S1).

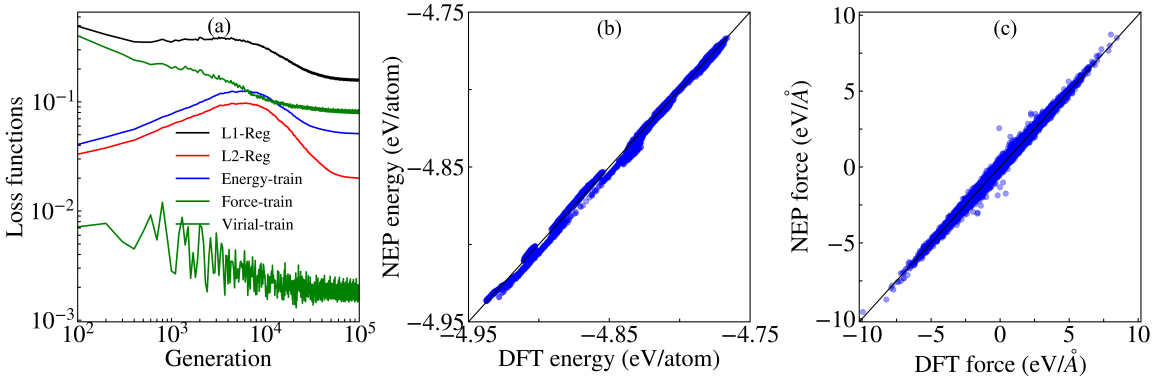

FIG. S1. (a) Evolution of the loss functions for L1-regression, L2-regression, energy, force, and virial during the training process. (b) The comparison of potential energy between DFT calculations and NEP based predictions for the test set. (b) The comparison of atomic forces between DFT calculations and NEP based predictions for the test set.

S2. Direct MD simulations

All MD simulations are carried out using the LAMMPS [7] and GPUMD [6] packages with a time step of 0.25 fs. LAMMPS is performed with the TIP4P model [8] and GPUMD with the NEP model. The system of water for MD calculations containing 2000 molecules with 6000 atoms is used for our MD simulations. After the structure relaxation and thermal equilibration in the isothermal-isobaric (NPT) ensemble under atmosphere pressure for 750 ps, EMD simulations with the microcanonical (NVE) ensemble are performed to record the atomic trajectories. A simulation time of 3 ns is used for the thermal conductivity calculations which is sufficient to ensure the convergence.

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