

Supplementary Materials for Neural Network Potential for Dislocation Plasticity in Ceramics

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S1 Supplementary information for main text

S1.1 SrTiO₃ [001] compression

A SrTiO₃ bulk model, measuring 24.2 nm × 24.2 nm × 24.2 nm and consisting of approximately 1.2 million atoms, was constructed (see Fig. S4a). The models are periodic in all three directions. The model was relaxed using the NPT ensemble at a temperature of 300 K and a timestep of 0.001 ps for 50 ps to release the stresses of model. Subsequently, a uniaxial compressive load was applied by linearly rescaling the system length in the [001] direction at a constant strain rate of $5 \times 10^8 \text{ s}^{-1}$ in an NPT ensemble at 300 K. Fig. S4b illustrates the snapshots of the dislocation structures under a compressive engineering strain of $\varepsilon = -0.10$. The $\{110\}\langle 1\bar{1}0 \rangle$ slip system is activated, and the dislocations slip on the $\{110\}$ plane, in good agreement with experimental results [1].

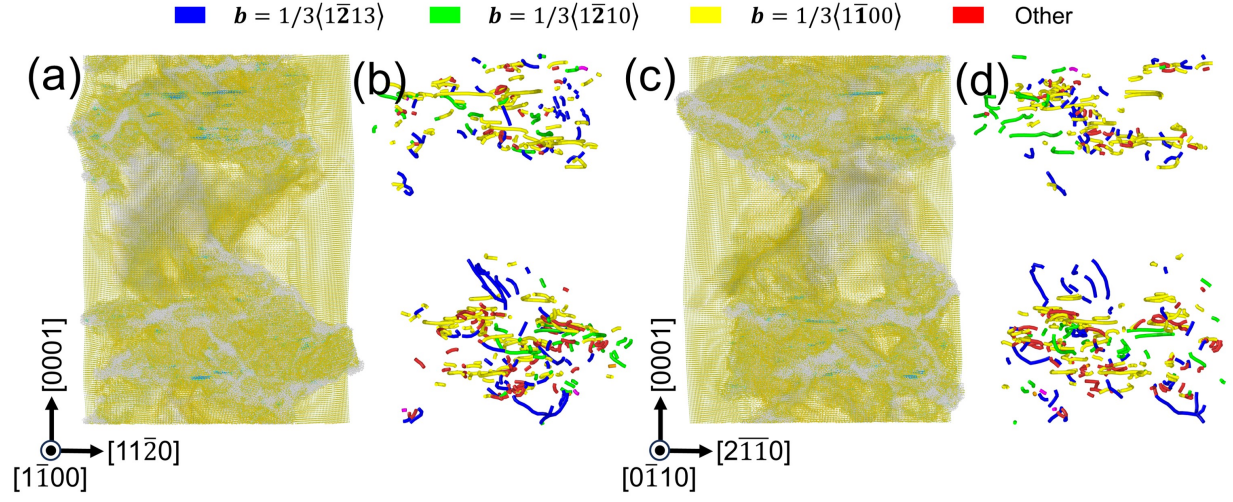


Figure S1: Snapshots of atomic configurations in the compression molecular dynamics (MD) simulation of *c*-oriented GaN nanopillar via SW empirical potential [2] under a compressive engineering strain $\varepsilon = -0.1940$ projected along (a-b) $[1\bar{1}00]$ and (c-d) $[0\bar{1}10]$, which were analyzed via (a, c) Identify Diamond Structure (IDS) method [3], and (b, d) Dislocation Extraction Algorithm (DXA) [4] based on Ga HCP sublattice. Atoms with a perfect wurtzite structure are not shown in (a,c).

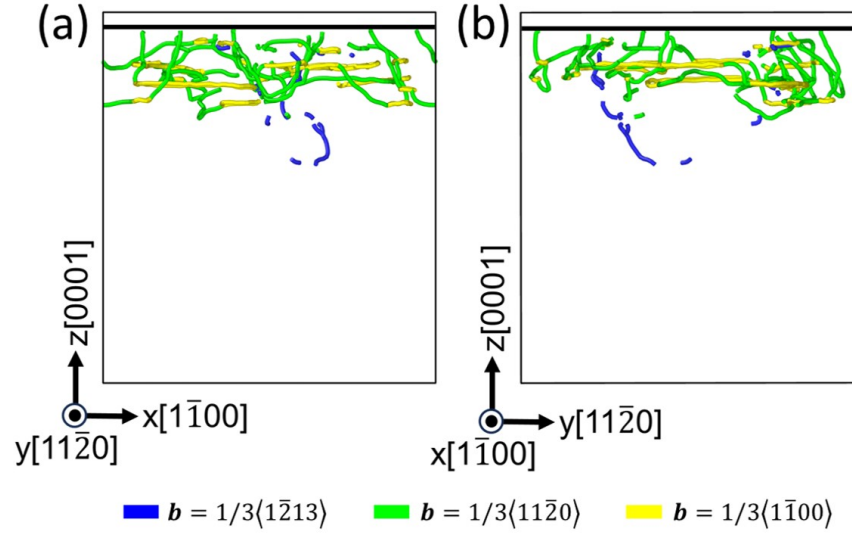


Figure S2: Snapshot of dislocation structures in the ZnO (0001) nanoindentation MD simulation via Buckingham-type empirical potential [5] as the indentation depth $h = 5.0$ nm projected along (a) $[11\bar{2}0]$, and (b) $[1\bar{1}00]$. The simulation parameters are the same as those used in the nanoindentation simulation via NNP.

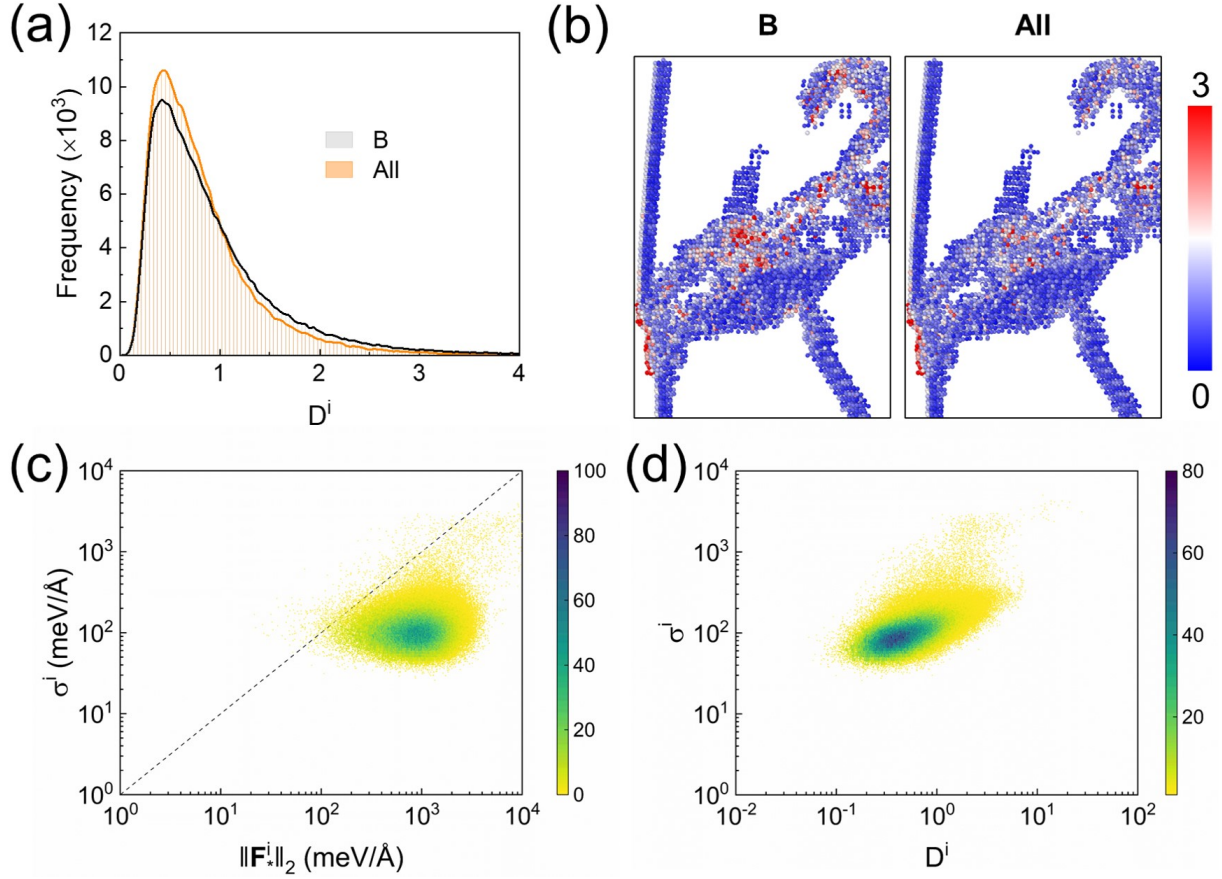


Figure S3: Similarity and uncertainty for atoms in the snapshot of c -oriented GaN nanopillar compression simulation under a compressive engineering strain of $\varepsilon = -0.1164$. (a) The distribution of similarity quantified by D^i with reference to the dataset consisting solely of basic structures ('B') and the comprehensive dataset ('All') which includes both the basic and dislocation-related structures. Only the atoms within the defected structures are shown. (b) Zoom-in of a portion of the defected structure, with atoms color-coded according to the value of D^i . The scatter plot of the uncertainty σ^i and (c) the magnitude of atomic force $\|\mathbf{F}_*^i\|_2$ and (d) the D^i for atoms within the defected structure in the snapshot. $\mathbf{F}_*^i$ represents the atomic force vector predicted by the NNP used to perform the compression simulation. The points are color-coded according to the value frequencies in each bin, with a bin size of (c) $[5, 5]$ and (d) $[0.0030, 5]$.

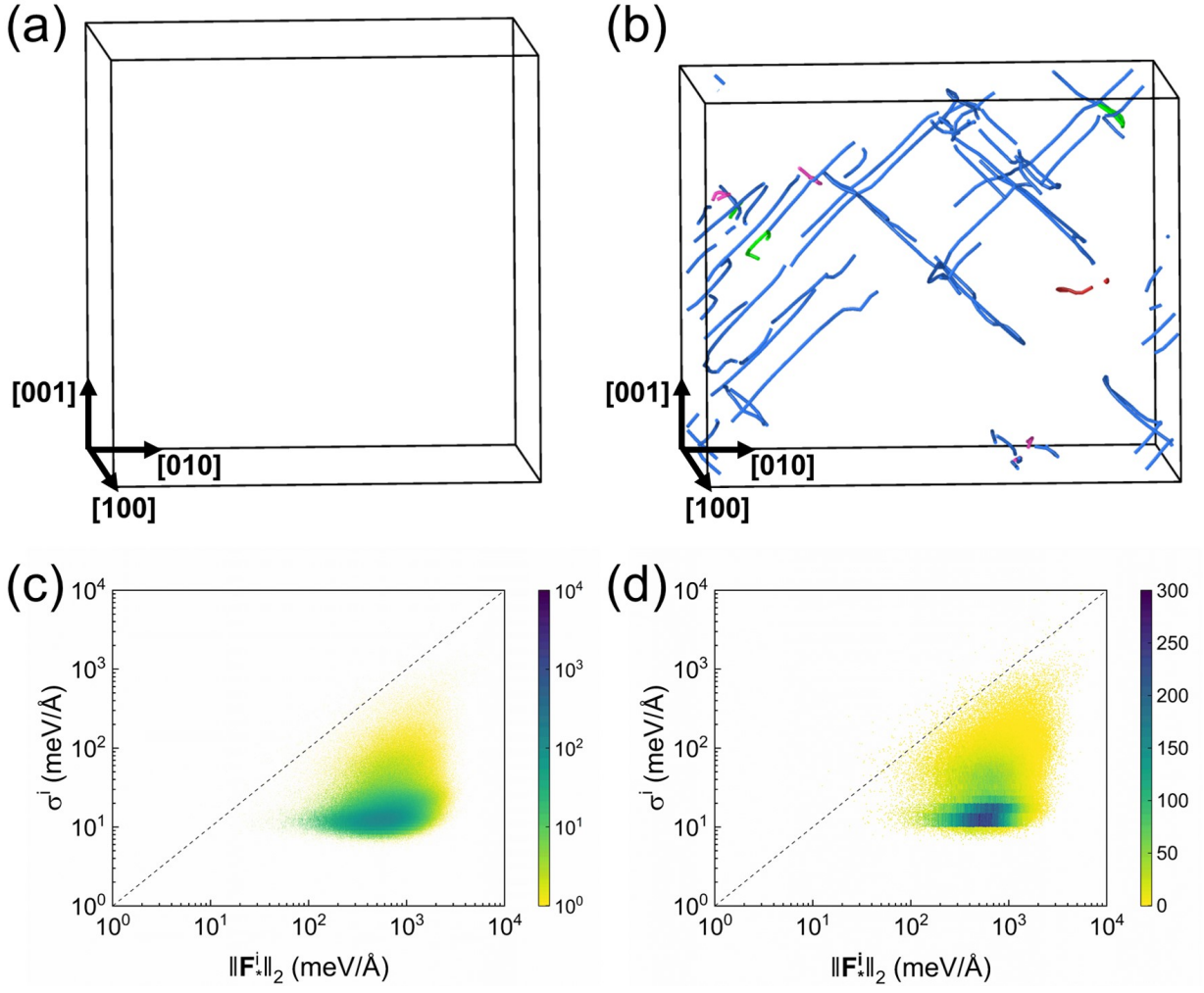


Figure S4: (a-b) Snapshot of dislocation structure in the SrTiO₃ [001] compression simulation under a compressive engineering strain of (a) $\varepsilon = 0.00$ and (b) $\varepsilon = -0.10$. The dislocation structures were analyzed based on the Sr-Ti BCC sublattice via the dislocation extraction algorithm (DXA) [4]. (c-d) The scatter plot of the uncertainty σ^i and the magnitude of atomic force $\|\mathbf{F}_*^i\|_2$ for (c) all atoms and (d) only atoms within the defected structure in the snapshot shown in (b). $\mathbf{F}_*^i$ represents the atomic force vector predicted by the NNP used to perform the compression simulation. The points are color-coded according to the value frequencies in each bin, with a bin size of (c) [1,1] and (d) [5,5].

Table S1: Training parameters, the number of DFT structures in training dataset, the root mean square error (RMSE) for energy and atomic force, as well as the value of the parameters η , ζ , r_s and θ_s selected in this work to determine the similarity quantified by D^i .

Parameter	ZnO	GaN	SrTiO ₃
Cutoff radius r_{cut} (Å)	7.0	7.0	6.0
Configuration of embedding net	{25, 50, 100}	{20, 40, 80}	{160, 160, 480}
Number of axis neurons	16	16	12
Configuration of fitting net	{240, 240, 240}	{200, 200, 200}	{240, 240, 240}
Initial learning rate	1.0×10^{-3}	1.0×10^{-3}	1.0×10^{-3}
Final learning rage	2.2×10^{-8}	2.2×10^{-8}	2.2×10^{-8}
Training step	1×10^6	3×10^6	3×10^6
Prefactors of energy weight p_e^{start}	0.02	0.01	0.02
Prefactors of energy weight p_e^{limit}	20	20	2
Prefactors of force weight p_f^{start}	1000	1000	1000
Prefactors of force weight p_f^{limit}	1	1	1
Number of DFT structures	13251	17686	7066
RMSE of energy (meV/atom)	3.5	5.5	2.5
RMSE of atomic force (meV/Å)	57.2	84.7	89.6
η in G_i^{rad}	1.0	1.0	1.0
r_s in G_i^{rad}	From 0 to 7.0 in steps of 0.25	From 0 to 7.0 in steps of 0.25	From 0 to 6.0 in steps of 0.25
ζ in G_i^{ang}	0.5	0.5	0.5
θ_s in G_i^{ang}	From 0 to 2π in steps of $\pi/6$	From 0 to 2π in steps of $\pi/6$	From 0 to 2π in steps of $\pi/6$
r_s in G_i^{ang}	From 0 to 7.0 in steps of 0.7	From 0 to 7.0 in steps of 0.70	From 0 to 6.0 in steps of 0.60

S2 Neural network potential of ZnO

S2.1 Detail of training dataset

The detail of the training dataset for the ZnO NNP is shown in Table S2. Three typical ZnO polymorphs were considered, including cubic rocksalt (B1), cubic zinc blende (B3), and hexagonal wurtzite (B4), shown in Fig. S5.

S2.2 Equilibrium structure

Fig. S6 shows the comparison of DFT and NNP predicted energies and components of atomic forces along x -, y - and z -axes of the structures in the training dataset. The root mean square errors (RMSEs) of ZnO NNP for energy and atomic force are 3.5 meV/atom and 57.2 meV/Å, respectively.

As shown in Table S3, we firstly compared the NNP and DFT predicted lattice constants, elastic constants, polycrystalline bulk and shear moduli, as well as the relative energy to B4-ZnO. The elastic constants of ZnO were determined via the AELAS code [6], and the polycrystalline bulk and shear moduli were calculated using the Voigt-Reuss-Hill approximation [7, 8]. The NNP predicted lattice constants are $a = 4.630$ Å of B3-ZnO, $a = 4.337$ Å of B1-ZnO, and $a = 3.287$ and $c = 5.305$ Å of B4-ZnO, which are very close to the DFT predicted value of 4.629, 4.338, 3.287, and 5.306 Å in this work, as well as 4.616, 4.328, 3.278, and 5.291 Å in Ref. [9], respectively. The NNP and DFT determined results also agree well with the experimental data of $a = 4.47$ Å for B3-ZnO, and $a = 3.25$ and $c = 5.21$ Å for B4-ZnO [10, 11]. The NNP determined shear and bulk moduli for B4-ZnO are 43.42 GPa and 129.17 GPa which are in reasonable agreement with the DFT results of 41.22 GPa and 129.59 GPa, respectively. The NNP calculated shear (bulk) moduli of B3-ZnO and B1-ZnO are 40.15 (124.73) and 61.46 (166.81) GPa, which agree well with the DFT results of 40.03 (129.41) and 62.85 (166.43) GPa, respectively. In addition, the NNP determined relative energies to B4-ZnO are 13.57 and 297.33 meV/f.u. for B3-ZnO and B1-ZnO, which are in excellent agreement with the DFT results of 14.32 and 297.15 meV/f.u., respectively.

We carried out short MD simulations of B3-ZnO, B1-ZnO, and B4-ZnO at various temperatures of 10, 20, 30, 60, 100, 200, 300, 600, 1000, 1500 and 2000 K over 1000 fs with a timestep of 1 fs. The snapshot structures were extracted every 20 MD step, and computed

using DFT for validation. Figs. S7a-b present the NNP and DFT predicted energies per atom and atomic forces of a total of 1650 extracted structures, for which the RMSEs of NNP results relative to DFT data are 3.9 meV/atom and 46.6 meV/Å for energies and atomic forces, respectively. Fig. S7c highlights the NNP predicted energies of B4-ZnO along the same MD trajectory at 300 K in comparison with their DFT reference, showing that no energy deviates from the DFT references by more than 2.0 meV/atom for B4-ZnO at 300 K. Furthermore, as shown in Fig. S7d, the majority of NNP force vectors are within 5° of their DFT references. Our NNP of ZnO catches the course of the energy and atomic force well, and we get near DFT accuracy in these simulations using this NNP.

The NNP performance for the phonon dispersion of B3-ZnO, B1-ZnO, and B4-ZnO compared with the DFT results are shown in Fig. S8. The phonon dispersion curve was calculated via a combination of phonoLAMMPS [12] and PHONOPY [13]. The NNP-predicted phonon dispersion curves of ZnO show a reasonable agreement with the DFT results. In addition, the absence of imaginary modes in the whole Brillouin zone confirms these three types of ZnO to be dynamically stable.

S2.3 Elastic deformation

Figs. S9a-b illustrate the NNP determined energy of B4-ZnO as a function of volumetric strain $\Delta V/V_0$ with or without Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion [14], as well as the DFT results for comparison. The ZBL repulsion only works as $\Delta V/V_0 < -0.50$, which can supply the shortage of NNP as describing the very close atom pairs. Together with the ZBL repulsion, the NNP describes well the deformation of B4-ZnO at a wide range of strain $\Delta V/V_0$ from -0.8 to 20.0 . The agreement to DFT results provides a validation of NNP accuracy. Fig. S9c shows the energy per atom as a function of the cell volume of different ZnO polymorphs: wurtzite (B4), Zinc blende (B3), NaCl (B1) and CsCl (B2), comparing with the DFT reference energies. The results of B2-ZnO are also

shown for comparison. It is noted that the results of B2-ZnO are NOT included in the training data. The NNP results show a good agreement with the DFT results.

S2.4 Cleavage and surface

Fig. S10 shows the NN performance for the binding energy $\chi(d)$ as a function of cleavage opening d without relaxation together with the DFT results for comparison. An agreement is obtained for the binding energy $\chi(d)$ and rigid cleavage energy $\chi_C \equiv \lim_{d \rightarrow \infty} \chi(d)$ of three types of ZnO, indicated the successful implementation of our NNP for the cleavage failure of ZnO.

Table S4 lists the NNP and DFT predicted surface energy of ZnO, which is defined as $(E_s - E_0)/A_s$, where E_s and E_0 are the energies of the surface structure and perfect structure, respectively, and A_s is the area of the surface. The NNP calculated surface energy are 3.01, 0.91, 4.91, 1.64, 0.61, 1.23, 3.12, 5.08, 1.65, 2.36, 0.94, and 0.92 J/m², which are similar with the DFT results of 3.00, 0.87, 5.00, 1.72, 0.56, 1.26, 3.27, 5.34, 1.95, 2.45, 1.04, and 0.88 J/m² for the (001), (011), (111) glide-set, and (111) shuffle-set planes of B3-ZnO, (001), (011), and (111) planes in B1-ZnO, as well as (0001) glide-set, (0001) shuffle-set, (10 $\bar{1}$ 0) glide-set, (10 $\bar{1}$ 0) shuffle-set, and (11 $\bar{2}$ 0) planes in B4-ZnO, respectively. The surface energy without relaxation, which corresponds to half of the rigid cleavage energy χ_C [15], is also shown in Table S4.

S2.5 Planar defect

The NNP performance for planar defects was also validated, including the twin, stacking fault (SF) and coherent heterophase interface for B3-ZnO, the twin (Zn-core), twin (O-core) and SF for B1-ZnO, as well as the I₁, I₂, I₃ and E types of SF, and the inversion domain boundary (IDB) of (10 $\bar{1}$ 0), (11 $\bar{2}$ 0) and (0001) planes for B4-ZnO as shown in Figs. S11 and

[S12](#). These planar defects have been widely observed in ZnO [16, 17, 18, 19, 20]. The NNP and DFT predicted formation energy of planar defects in ZnO defined as $(E_d - E_0)/A_d$ are listed in Table [S5](#), where E_d and E_0 are the energies of the structure consisting of planar defect and the perfect structure, respectively, and A_d is the area of the planar defect. The NNP determined formation energy of planar defects are -0.05 , -0.09 , -0.14 , 1.26 , 0.65 , 1.77 , 0.05 , 0.09 , 0.14 , 0.09 , 0.22 , 0.27 , 4.9 , and 2.14 J/m² for the planar defects of twin, SF, and coherent heterophase interface in B3-ZnO, twin (Zn), twin (O) and SF planar defects in B1-ZnO, as well as I₁-SF, I₂-SF, I₃-SF, E-SF, IDB-(10 $\bar{1}$ 0) I, IDB-(11 $\bar{2}$ 0), IDB-(0001) and IDB-(10 $\bar{1}$ 0) II planar defects in B4-ZnO, which agree well with the DFT results of -0.05 , -0.13 , -0.13 , 1.23 , 0.63 , 1.73 , 0.06 , 0.06 , 0.15 , 0.06 , 0.25 , 0.26 , 5.88 , and 2.01 J/m², respectively.

S2.6 Stacking fault

Fig. [S13](#) shows the NNP performance for the generalized stacking fault energies of B4-ZnO compared with the DFT results. The typical slip systems on the basal (0001), prismatic I (10 $\bar{1}$ 0), prismatic II (11 $\bar{2}$ 0), pyramidal I (10 $\bar{1}$ 1), and pyramidal II (11 $\bar{2}$ 2) planes in the hexagonal close packing (HCP) structure are considered. Especially, in the wurtzite (B4) structure, there include two different slip planes, i.e., glide-set and shuffle-set, on basal (0001) and prismatic I (10 $\bar{1}$ 0) planes (see Fig. [S14](#)). It is noted that the results of pyramidal I and II planes are NOT included in the training data. The NNP-predicted generalized stacking fault energies are in good agreement with the DFT results, which provides a solid foundation for the simulation of the dislocation-dominant deformation in B4-ZnO using this NNP since the stacking fault energy is a fundamental property for the dislocation nucleation and slip [21, 22]. The NNP-determined generalized stacking fault energies of B3-ZnO are shown in Fig. [S15](#), which also agree well with the DFT results.

S2.7 Dislocation

Figs. S16 and S17 show the dislocation structures of basal shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, $1/3\langle 11\bar{2}0 \rangle$ screw dislocation, and basal glide-set $1/3\langle 1\bar{1}00 \rangle$ partial dislocations in B4-ZnO. In the case of the basal glide-set $1/3\langle 1\bar{1}00 \rangle$ edge partial dislocation, the core can be reconstructed into the double period (DP) structure (see Figs. S17c-d) to eliminate dangling bonds comparing to the single period (SP) structure (see Figs. S17a-b). Their Peierls barriers calculated via NNP and DFT are shown in Fig. S18, which were determined via the dislocation dipole model of quadrupolar arrangement and the NEB method. To be noted that except the prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, $1/3\langle 11\bar{2}0 \rangle$ screw dislocation, and basal glide-set $1/3\langle 1\bar{1}00 \rangle$ partial screw dislocation, the calculated Peierls barrier of other dislocations is an average value of those with O core and Zn core shown in Figs. S16 and S17. Different simulation cell size was used, which is defined by the number of (n,m) . The NNP results have a great agreement with the DFT results.

Figures

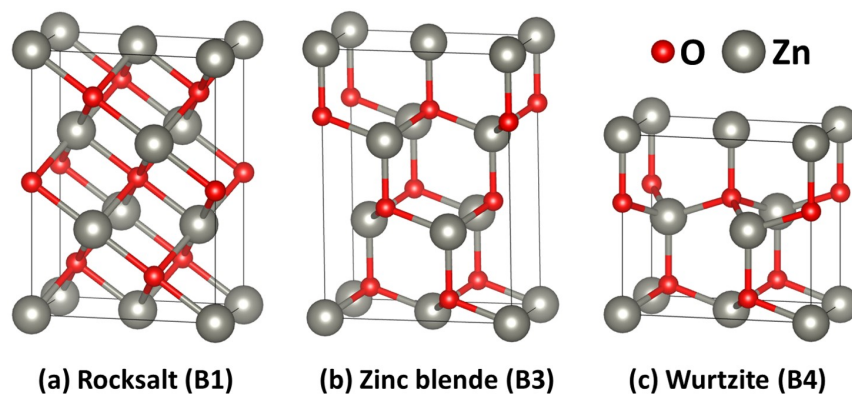


Figure S5: Stick and ball representation of typical ZnO polymorphs: (a) cubic rocksalt (B1), (b) cubic zinc blende (B3), and (c) hexagonal wurtzite (B4).

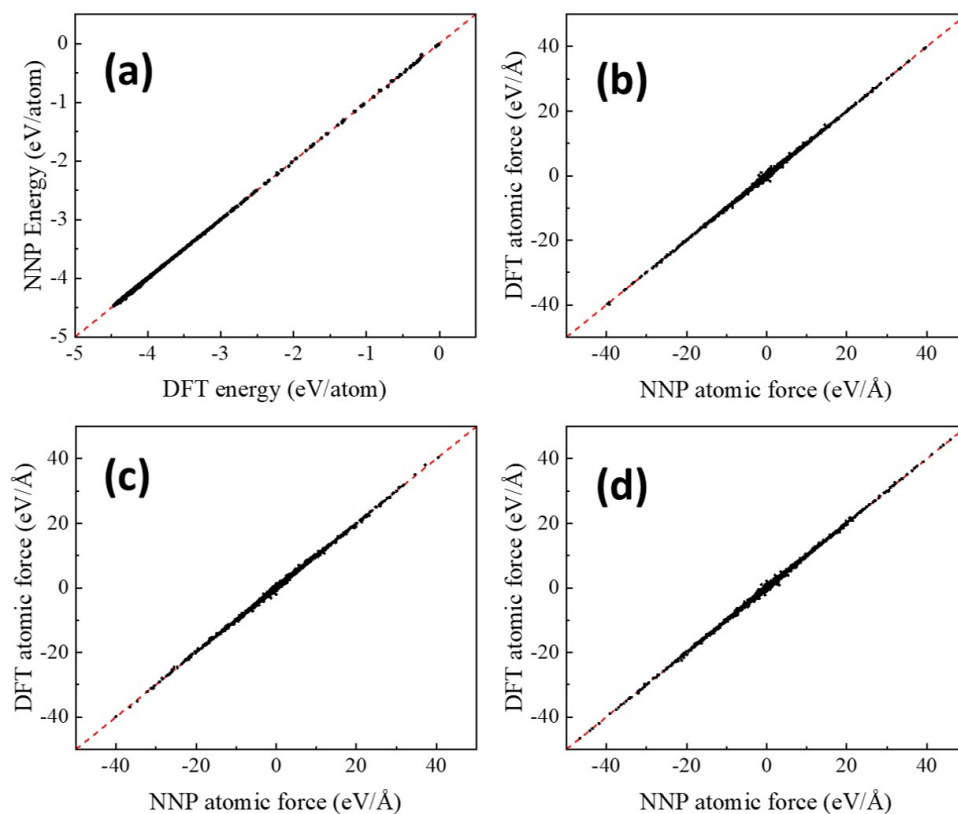


Figure S6: Comparison of DFT and NNP predicted (a) energies and (b-d) components of atomic forces along (b) x -, (c) y - and (d) z -axes of the structures in the training dataset. The line with a slope of 1 corresponds to perfect training.

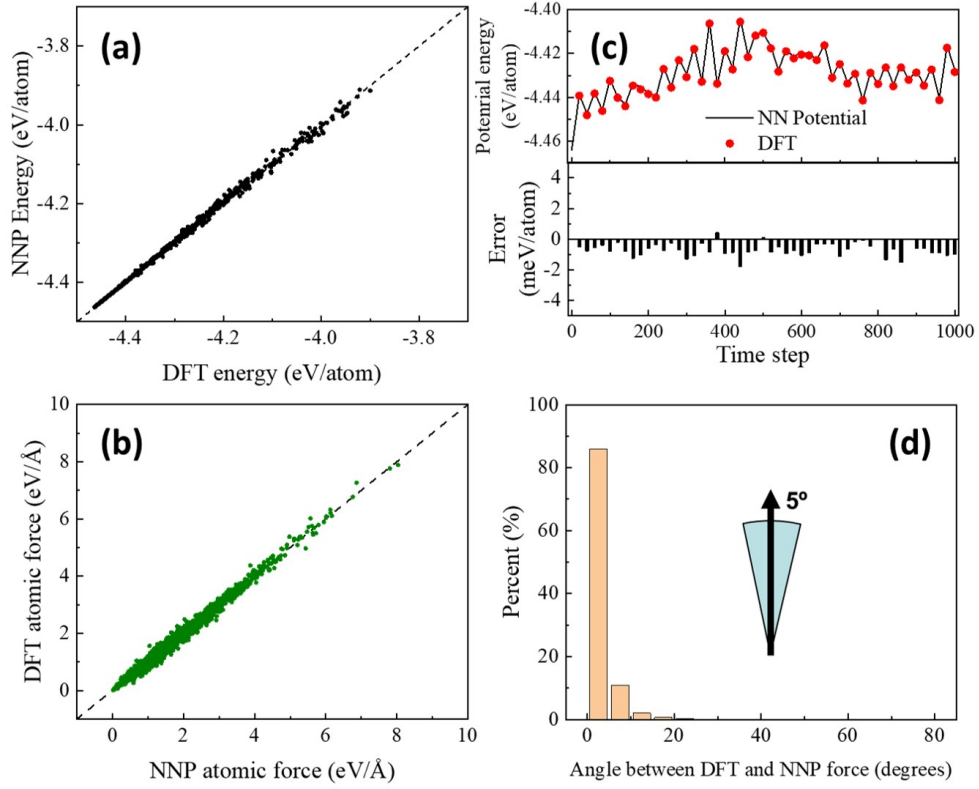


Figure S7: Comparison of the NNP and DFT predicted (a) energies and (b) atomic forces of the extracted structures from a 1000 fs MD trajectory with a time step of 1 fs under different temperatures of 10, 20, 30, 60, 100, 200, 300, 600, 1000, 1500, and 2000 K. The snapshot structures were extracted every 20 MD steps. (c) Energy of B4-ZnO predicted by the NNP and DFT calculations along the same MD trajectory at 300 K. (d) Histogram of the absolute directional errors in the NNP prediction of the atomic force. The majority of NNP force vectors are within 5° of their DFT references; this trust region is depicted as the blue area in the inset.

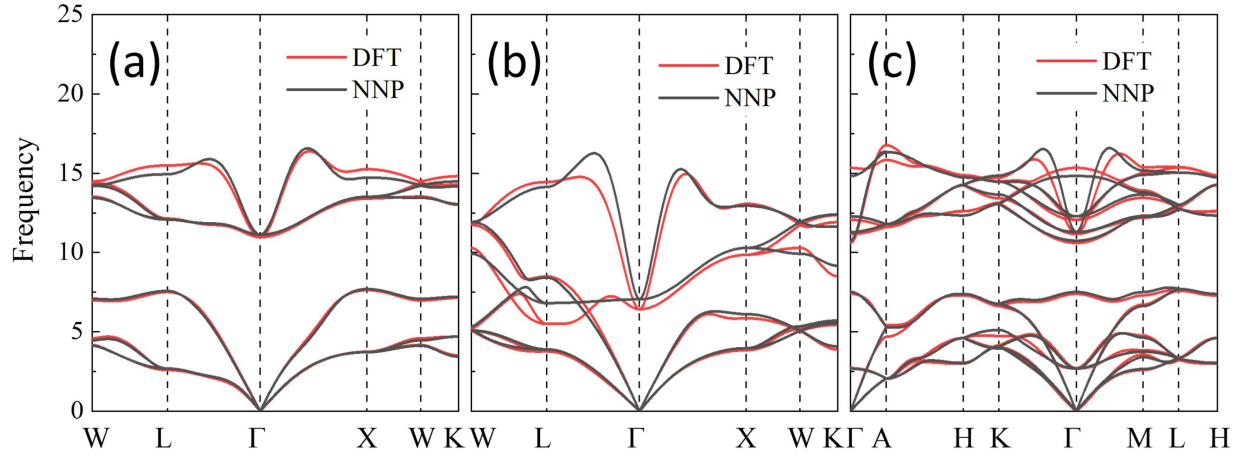


Figure S8: NNP performance for the phonon dispersion of (a) B3-ZnO, (b) B1-ZnO and (c) B4-ZnO, comparing with the DFT results.

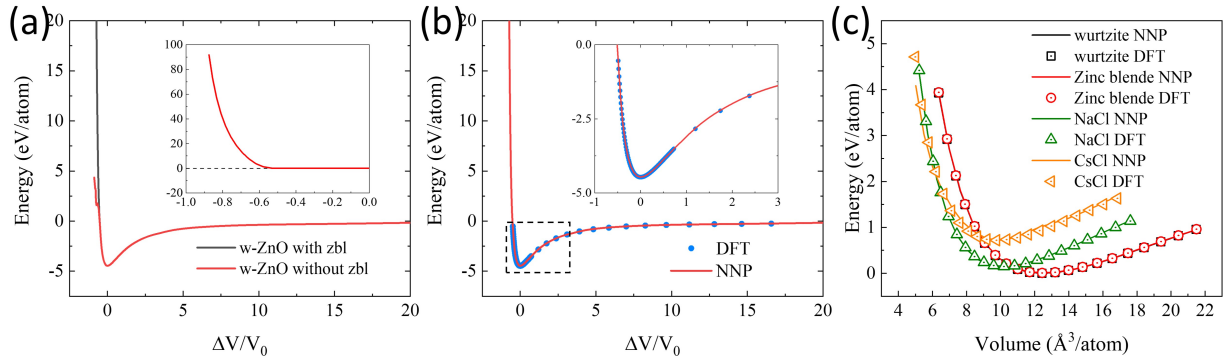


Figure S9: (a-b) The energy of B4-ZnO as a function of volumetric strain $\Delta V/V_0$ with or without Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion, as well as the DFT results for comparison. (Insert) The energy resulting from the ZBL repulsion is shown in (a). (c) Energy per atom as a function of the cell volume for the ZnO crystal polymorphs: wurtzite (B4), Zinc blende (B3), NaCl (B1), and CsCl (B2). Symbols correspond to the DFT reference energies and lines interpolate the NNP predicted energies. The results of B2-ZnO are also shown for comparison. It is noted that the results of B2-ZnO are NOT included in the training dataset.

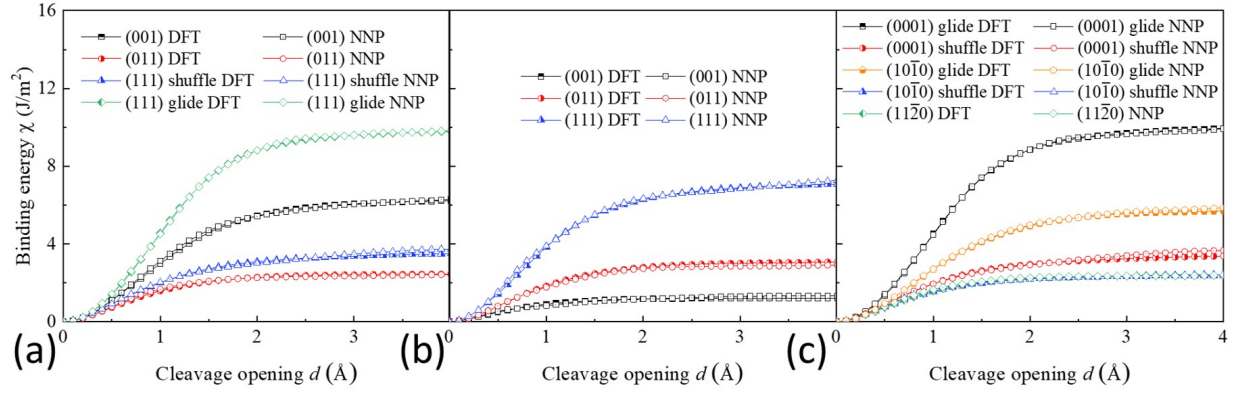


Figure S10: NNP performance for the binding energy as a function of cleavage opening d without relaxation: (a) B3-ZnO, (b) B1-ZnO and (c) B4-ZnO, together with the DFT results for comparison.

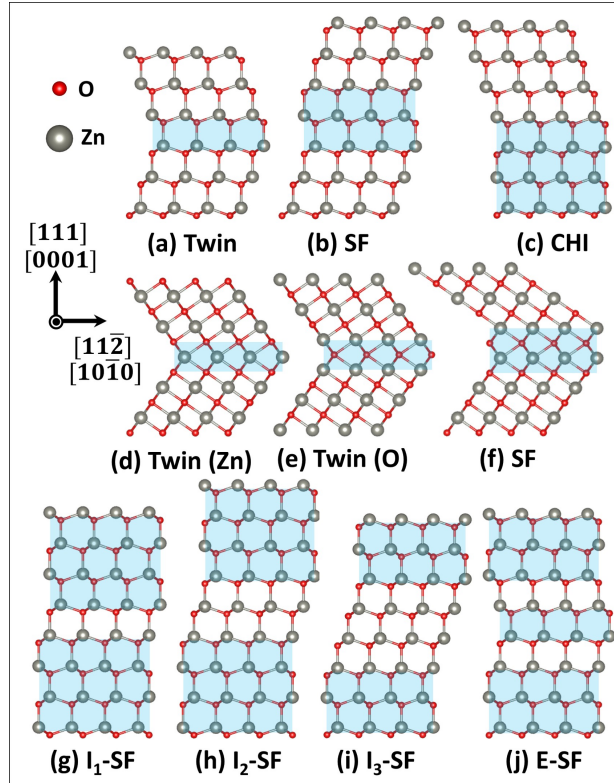


Figure S11: (a-c) Twin, stacking fault (SF) and coherent heterophase interface (CHI) in B1-ZnO, (d-f) twin (Zn), twin (O) and SF in B3-ZnO, as well as (g-j) the I_1 , I_2 , I_3 and E types of SF in B4-ZnO.

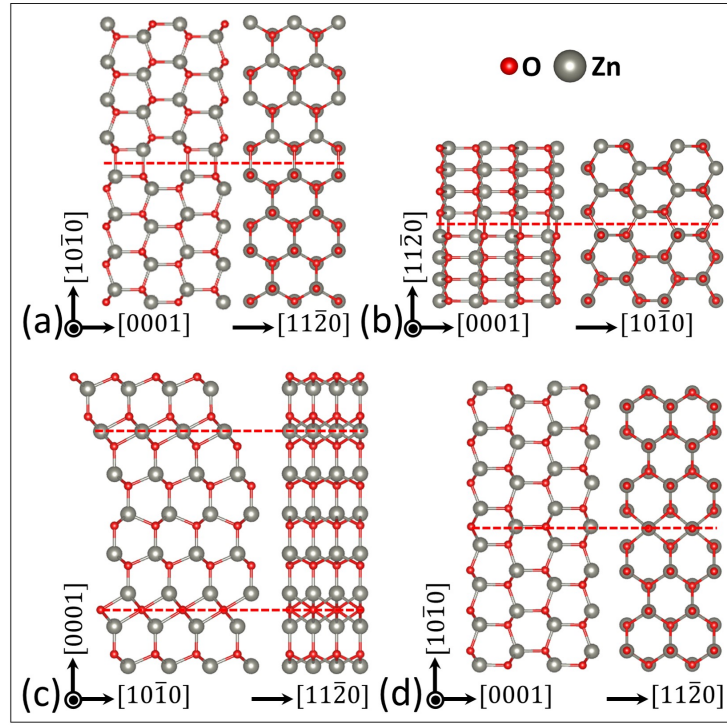


Figure S12: The inversion domain boundary (IDB) of (10 $\bar{1}$ 0), (11 $\bar{2}$ 0) and (0001) planes in B4-ZnO: (a) IDB-(10 $\bar{1}$ 0) I, (b) IDB-(11 $\bar{2}$ 0), (c) IDB-(0001), and (d) IDB-(10 $\bar{1}$ 0) II.

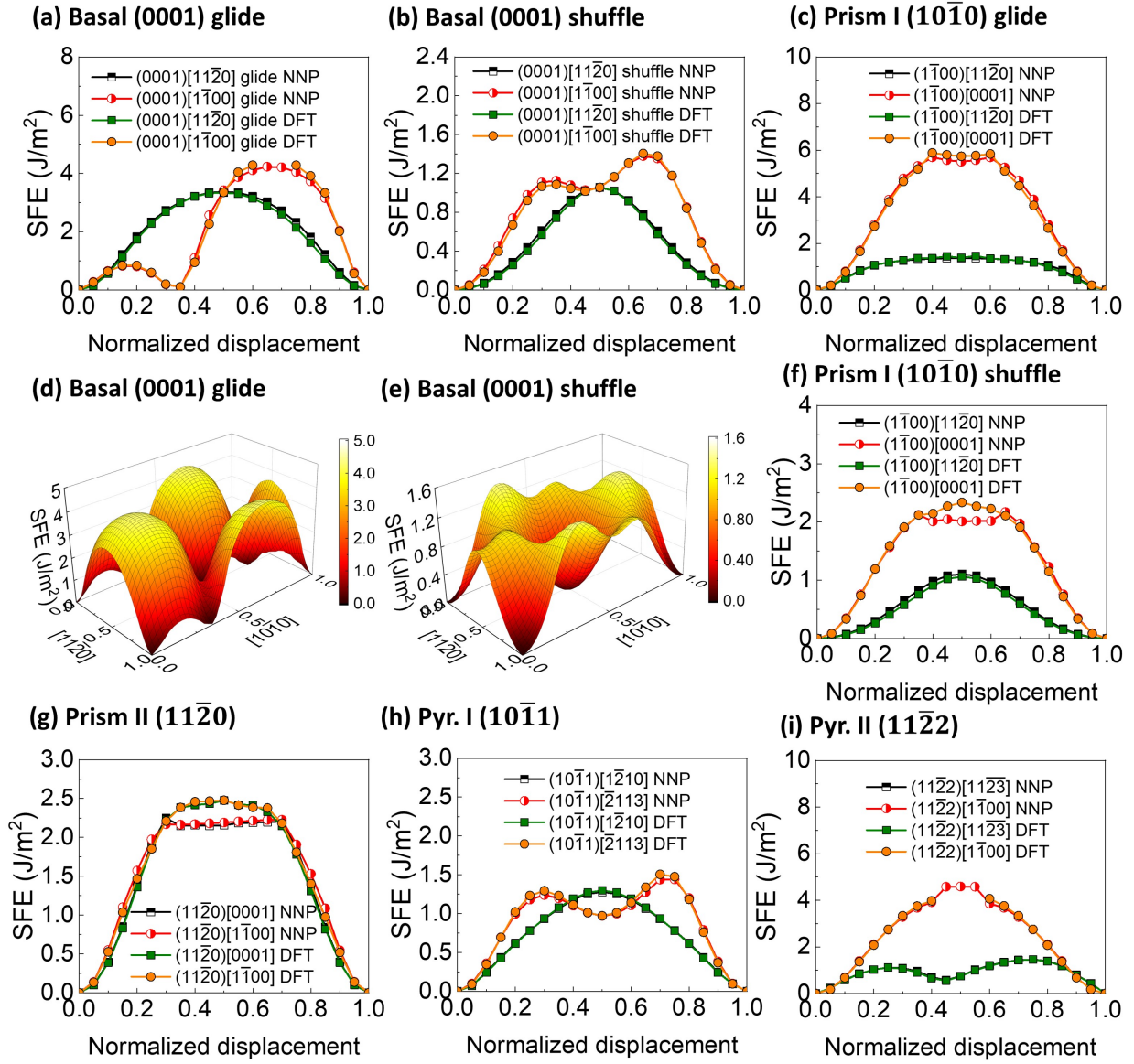


Figure S13: NNP performance for the generalized stacking fault energy of B4-ZnO comparing with the DFT results. The orientation of the basal and prismatic I planes of shuffle-set and glide-set are shown in Fig. S14.

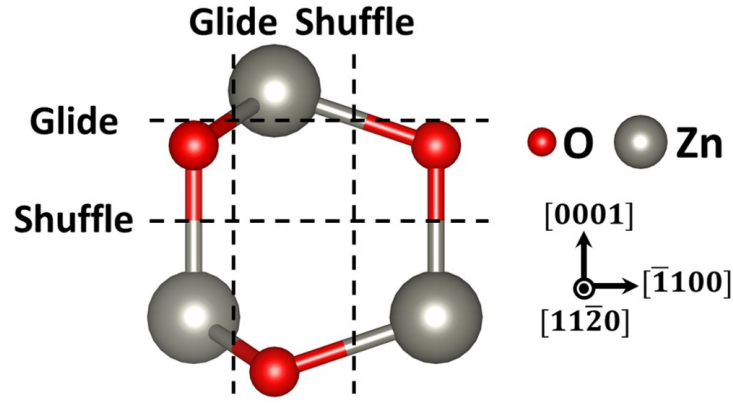


Figure S14: Basal and prismatic I planes of shuffle-set and glide-set in wurtzite structure.

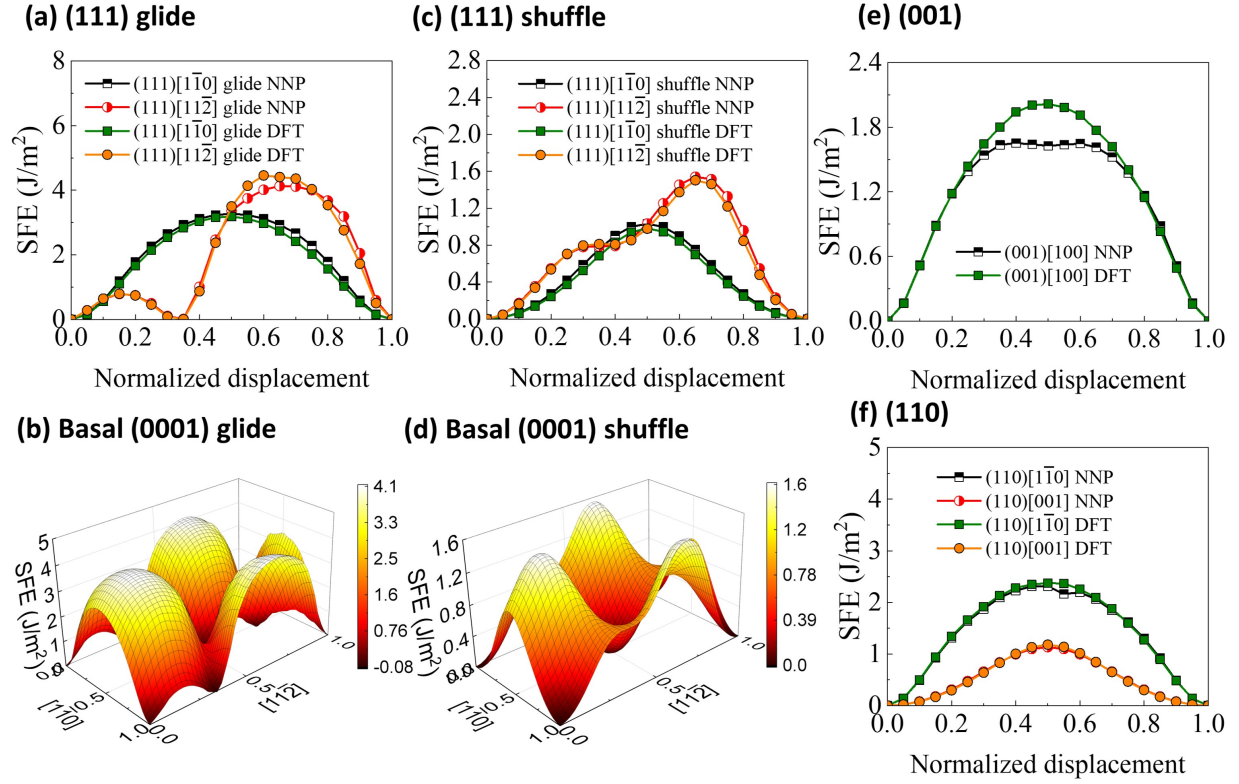


Figure S15: NNP performance for the generalized stacking fault energy of B3-ZnO comparing with the DFT results.

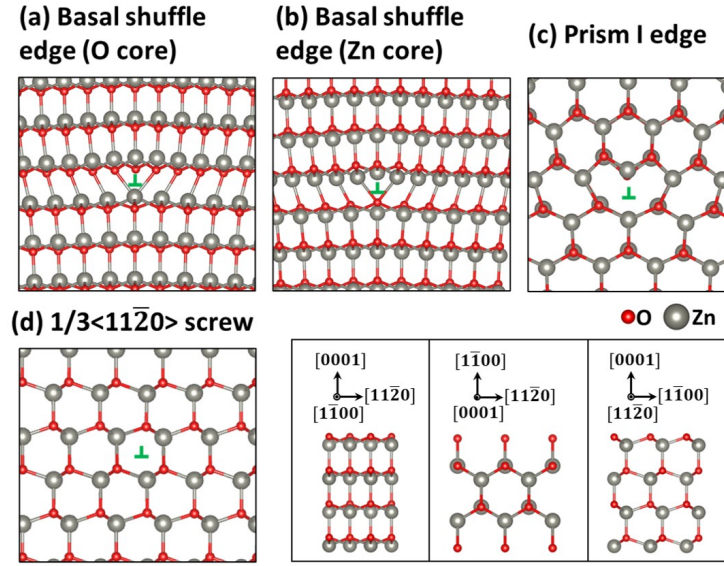


Figure S16: Dislocation structures of (a-b) basal shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation with O core and Zn core, (c) prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, and (d) $1/3\langle 11\bar{2}0 \rangle$ screw dislocation in B4-ZnO. All structures are viewed along the dislocation line direction. The positions of dislocation core are highlighted by grep “ $\perp$ ”.

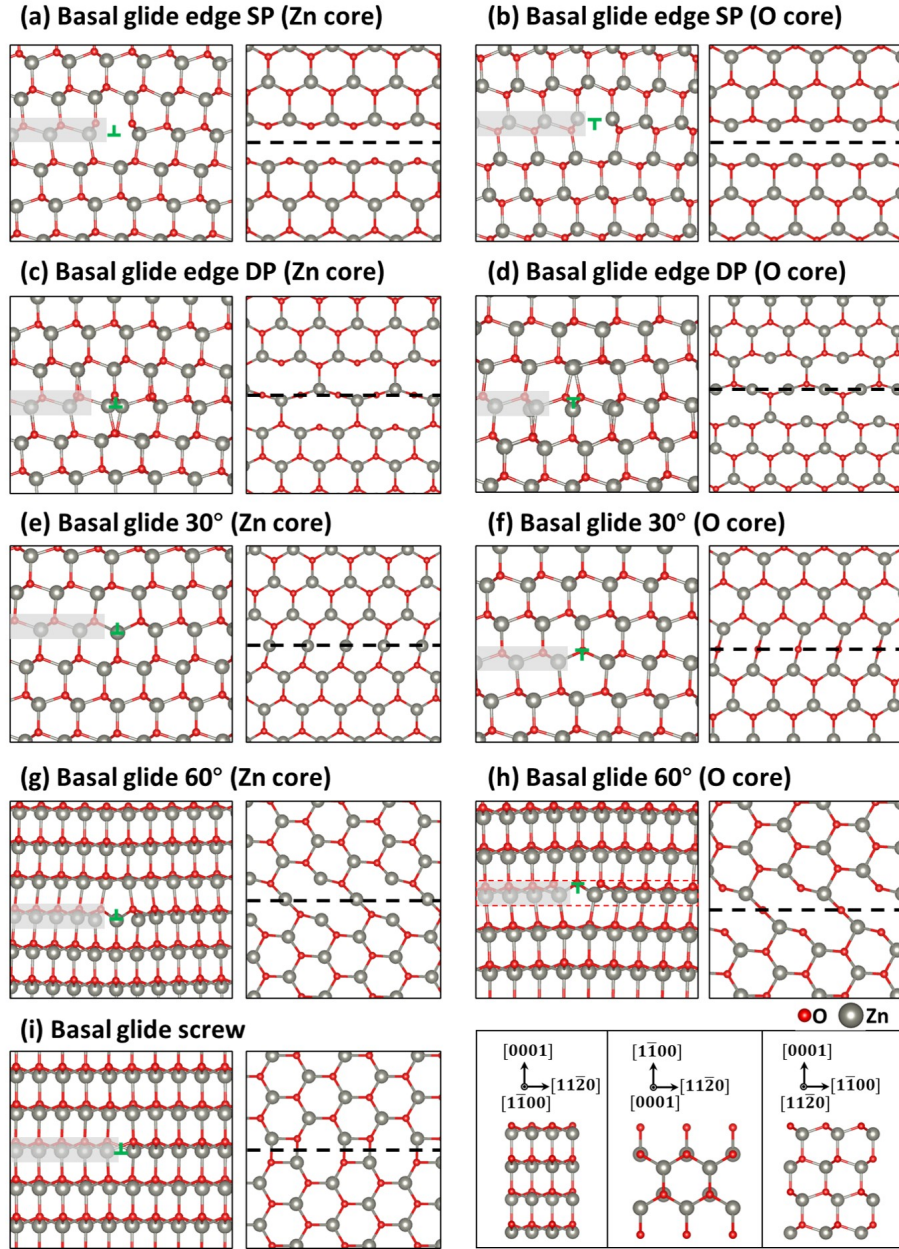


Figure S17: Dislocation structures of basal glide-set $1/3 \langle 1\bar{1}00 \rangle$ partial dislocations in B4-ZnO (left) viewed along the dislocation line direction and (right) viewed normal to the (0001) slip plane. Broken black lines indicate dislocation lines along the cores. The positions of the dislocation core are highlighted by grep “ $\perp$ ”. The stacking faults are highlighted by the gray region. In the case of the edge partial dislocation, the core can be reconstructed into the double period (DP) structure to eliminate dangling bonds compared to the single period (SP) structure.

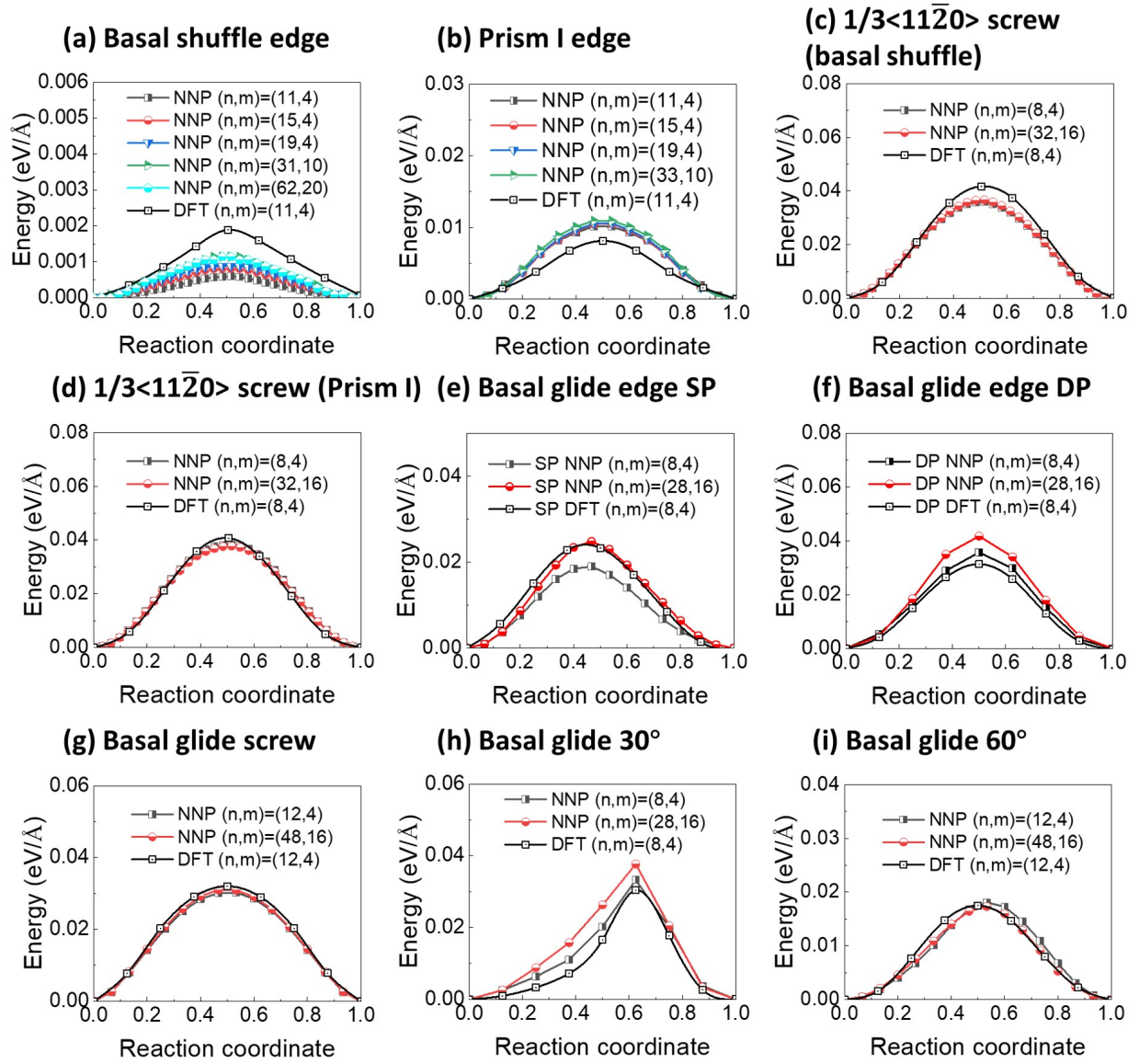


Figure S18: The Peierls barrier of (a) basal shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, (b) prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, $1/3\langle 11\bar{2}0 \rangle$ screw dislocation slipping on (c) basal and (d) prismatic I shuffle-set planes, as well as (e-i) basal glide-set $1/3\langle 1\bar{1}00 \rangle$ partial dislocations slipping on basal glide-set plane. They were calculated via the dislocation dipole model of quadrupolar arrangement and the NEB method. The DFT results are also shown for comparison. To be noted that except the prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, $1/3\langle 11\bar{2}0 \rangle$ screw dislocation, and basal glide-set $1/3\langle 1\bar{1}00 \rangle$ partial screw dislocation, the calculated Peierls barrier of other dislocations is an average value of those with O core and Zn core shown in Figs. S16 and S17.

Tables

Table S2: Training dataset employed to construct the NNP of ZnO, all of which were calculated via DFT calculations.

Type of str.	Description
Elastic deformation	• The deformation pattern of B3-ZnO and B1-ZnO: $(\varepsilon, 0, 0, 0, 0, 0)$, $(\varepsilon, \varepsilon, 0, 0, 0, 0)$, $(0, 0, 0, \varepsilon, 0, 0)$, $(0, 0, 0, \varepsilon, \varepsilon, 0)$, $(0, 0, 0, \varepsilon, \varepsilon, \varepsilon)$, $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$; • The deformation pattern of B4-ZnO: $(\varepsilon, 0, 0, 0, 0, 0)$, $(0, 0, \varepsilon, 0, 0, 0)$, $(\varepsilon, \varepsilon, 0, 0, 0, 0)$, $(\varepsilon, 0, \varepsilon, 0, 0, 0)$, $(0, 0, 0, \varepsilon, 0, 0)$, $(0, 0, 0, 0, 0, \varepsilon)$, $(0, 0, 0, \varepsilon, \varepsilon, 0)$, $(0, 0, 0, \varepsilon, 0, \varepsilon)$, $(0, 0, 0, \varepsilon, \varepsilon, \varepsilon)$, $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$; • The ranges of strain ε are $-0.20 \sim 1.60$ for the $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$ deformation pattern, and $-0.20 \sim 0.20$ for other types of deformation pattern; • Relaxation: No relaxation for both atomic position and cell shape.
Tensile, compress and shear loadings	• Direction of tensile and compress loadings: $[001]$, $[011]$ and $[111]$ for B3-ZnO and B1-ZnO, and $[0001]$, $[11\bar{2}0]$ and $[10\bar{1}0]$ for B4-ZnO; • Direction of shear loading: $(001)[100]$, $(001)[110]$, $(110)[001]$, $(110)[1\bar{1}0]$, $(111)[1\bar{1}0]$, $(111)[\bar{1}12]$ and $(111)[11\bar{2}]$ for B3-ZnO and B1-ZnO, and $(0001)[11\bar{2}0]$, $(0001)[10\bar{1}0]$ and $(10\bar{1}0)[0001]$ for B4-ZnO; • Strain range: from 0.00 to the strain where the failure occurs; • Relaxation: 1) Full relaxation of both atomic position and cell shape except the applied strain component; 2) No relaxation of both atomic position and cell shape.
Cleavage	• (001), (011) and (111) planes for B3-ZnO and B1-ZnO, and (0001), $(10\bar{1}0)$ and $(11\bar{2}0)$ planes for B4-ZnO; • Range of cleavage opening d: $0.0 \sim 4.0$ Å; • Relaxation: No relaxation for both atomic position and cell shape.
Surface	• (001), (011) and (111) planes for B3-ZnO and B1-ZnO, and (0001), $(10\bar{1}0)$ and $(11\bar{2}0)$ planes for B4-ZnO; • Thickness of vacuum layer: 15 Å; • Relaxation: 1) Relaxation of the positions of only the atoms whose distance away from surface smaller than 4 Å; 2) No relaxation of both atomic position and cell shape.
Vacancy	• Insert randomly 1 O, 1 Zn, 2 O, 2 Zn, 3 O or 3 Zn vacancies in the supercell structures consisting of 96 atoms for B3-ZnO and B1-ZnO, and 128 atoms for B4-ZnO; • Relaxation: 1) Full relaxation of both atomic position and cell shape; 2) No relaxation of both atomic position and cell shape.

Stacking fault	• (001)[010], (001)[100], (011)[100], (011)[01$\bar{1}$], (111)[1$\bar{1}$0] and (111)[11$\bar{2}$] for B3-ZnO and B1-ZnO, and (0001)[10$\bar{1}$0], (0001)[11$\bar{2}$0], (11$\bar{2}$0)[0001], (11$\bar{2}$0)[10$\bar{1}$0], (10$\bar{1}$0)[0001] and (10$\bar{1}$0)[11$\bar{2}$0] for B4-ZnO; • Relaxation: 1) Only the atomic movement normal to the slip plane together with cell shape are permitted to relax; 2) No relaxation of both atomic position and cell shape;
Twining	• Twinning along (111)[11$\bar{2}$] slip system for B3-ZnO and B1-ZnO; • Relaxation: 1) Only the atomic movement normal to the slip plane together with cell shape are permitted to relax; 2) No relaxation of both atomic position and cell shape.
Grain boundary	• Σ5 and Σ10 tilt grain boundaries for B3-ZnO, and • Σ5 tilt grain boundary for B1-ZnO; • Relaxation: Full relaxation of both atomic position and cell shape.
Planar defect	• (111) twin, (111) stacking fault, and coherent heterophase interface for B3-ZnO; • (111) twin, and (111) stacking fault for B1-ZnO; • I1, I2, I3 and extrinsic (E) basal-plane stacking faults, inversion domain boundary of (10$\bar{1}$0), (11$\bar{2}$0) and (0001) planes for B4-ZnO; • Relaxation: Full relaxation of both atomic position and cell shape.
Distortion	• Add different random distortions to each atom in the supercell of B3-ZnO, B1-ZnO and B4-ZnO to create the distorted structures; • Size of supercell: 1$\times$1$\times$1 unit cell and 2$\times$2$\times$2 supercell for B3-ZnO and B1-ZnO, as well as 2$\times$2$\times$1 and 3$\times$3$\times$2 supercells for B4-ZnO; • Atomic coordinate changes from (x, y, z) to $(x + dx, y + dy, z + dz)$, where dx, dy and dz are random values ranging from $-d^{max}$ to d^{max}; • d^{max} (in Å): 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.12, 0.15, 0.20 and 0.25.
Amorphous	• These amorphous structures are created as follows: 1) run 8000 fs with a timestep of 1 fs and a supercell consisting of 96 atoms at 6000 K via VASP AIMD; 2) Full relaxation of both atomic position and lattice constant.
Isolate atom	• The energy of isolate O or Zn atom is calculated; • Size of supercell: 10 Å$\times$10 Å$\times$10 Å, 20 Å$\times$20 Å$\times$20 Å, and 30 Å$\times$30 Å$\times$30 Å.

Table S3: NNP and DFT predicted lattice constant (a and c in Å), elastic constants (c_{ij} in GPa), the polycrystalline shear (μ) and bulk (κ) moduli (in GPa) calculated via the Voigt-Reuss-Hill approximation [7, 8], as well as the relative energy to B4-ZnO (ΔE in meV/f.u.). The theoretical values and experimental data previously published in the literature are also shown for comparison.

	a	c	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}	μ	κ	ΔE	Note
B4-ZnO	3.287	5.305	201	120	101	213	38	41	43.42	129.17	0.00	This work, NNP
	3.287	5.306	188	107	94	201	37	40	41.22	129.59	0.00	This work, GGA-PBE
	3.278	5.291										GGA-PBE [9]
			191.5	108.7	95	206.7	41.4	38				PBE [23]
			221.1	105.9	87.4	234.3	57.6	53.4				PBE+U [23]
	3.195	5.160										LDA [24]
	3.148	5.074										LDA+U [24]
	3.25	5.21										Exp [11]
			190	110	90	196	39	40				Exp. [11]
			206	117	118	211	44.3	44.6				Exp. [25]
B3-ZnO	4.630		161	126			70		40.15	124.73	13.57	This work, NNP
	4.629		155	116			64		40.03	129.41	14.32	This work, GGA-PBE
	4.616											GGA-PBE [9]
										161.7		LDA [27]
										135.3		GGA [27]
	4.47											Exp. [10]
B1-ZnO	4.337		232	167			84		61.46	166.81	297.33	This work, NNP
	4.338		223	138			82		62.85	166.43	297.15	This work, GGA-PBE
	4.328											GGA-PBE [9]
										172.7		GGA [27]
										202.5		Exp. [28]

Table S4: NNP and DFT predicted surface energy of ZnO (in J/m²). Both of the results without relaxation (which corresponds to half of the rigid cleavage energy [15]) and with full relaxation are shown.

	Surface	DFT (unrelaxed)	DFT (fully relaxed)	NNP (unrelaxed)	NNP (fully relaxed)
B3-ZnO	(001)	3.22	3.00	3.22	3.01
	(011)	1.21	0.87	1.22	0.91
	(111) Glide	5.13	5.00	5.04	4.91
	(111) Shuffle	2.02	1.72	1.86	1.64
B1-ZnO	(001)	0.60	0.56	0.69	0.61
	(011)	1.54	1.26	1.51	1.23
	(111)	3.93	3.27	3.76	3.12
B4-ZnO	(0001) Glide	5.47	5.34	5.24	5.08
	(0001) Shuffle	2.39	1.95	1.88	1.65
	(10 $\bar{1}$ 0) Glide	3.00	2.45	2.97	2.36
	(10 $\bar{1}$ 0) Shuffle	1.36	1.04	1.22	0.94
	(11 $\bar{2}$ 0)	1.19	0.88	1.20	0.92

Table S5: NNP and DFT predicted formation energy of planar defects in ZnO (in J/m²). The planar defects include twin, stacking fault (SF) and coherent heterophase interface (CHI) in B3-ZnO, twin (Zn), twin (O) and SF in B1-ZnO, as well as the I₁, I₂, I₃ and E types of SF, and the inversion domain boundary (IDB) of (10 $\bar{1}$ 0), (11 $\bar{2}$ 0) and (0001) planes in B4-ZnO (see Fig. [S11](#) and [S12](#)).

	Planar defect	DFT	NNP
B3-ZnO	Twin	-0.02	-0.02
	SF	-0.07	-0.05
	CHI	-0.07	-0.07
B1-ZnO	Twin (Zn)	0.62	0.63
	Twin (O)	0.31	0.32
	SF	0.86	0.89
B4-ZnO	I ₁ -SF	0.03	0.02
	I ₂ -SF	0.03	0.05
	I ₃ -SF	0.07	0.07
	E-SF	0.03	0.05
	IDB-(10 $\bar{1}$ 0) I	0.12	0.11
	IDB-(11 $\bar{2}$ 0)	0.13	0.14
	IDB-(0001)	2.94	2.45
	IDB-(10 $\bar{1}$ 0) II	1.00	1.07

S3 Neural network potential of GaN

S3.1 Detail of training dataset

The detail of the training dataset for the GaN NNP is shown in Table S6. Two typical GaN polymorphs were considered, including cubic zinc-blende (B3) and hexagonal wurtzite (B4), as shown in Fig. S19.

S3.2 Equilibrium structure

Fig. S20 shows the comparison of DFT and NNP predicted energies and components of atomic forces along x -, y - and z -axes of the structures in the training dataset. The root mean square errors (RMSEs) of GaN NNP for energy and atomic force are 5.5 meV/atom and 84.7 meV/Å, respectively.

As shown in Table S7, we firstly compared the NNP and DFT predicted lattice constants, elastic constants, polycrystalline bulk and shear moduli, as well as the relative energy to B4-GaN. The elastic constants of GaN were determined via the AELAS code [6], and the polycrystalline bulk and shear moduli were calculated using the Voigt-Reuss-Hill approximation [7, 8]. The NNP predicted lattice constants are $a = 4.580$ Å of B3-GaN, and $a = 3.224$ and $c = 5.290$ Å of B4-GaN, which are very close to the DFT predicted value of 4.588, 3.248, and 5.282 Å in this work, respectively. The NNP and DFT determined results also agree well with the experimental data of $a = 3.190$ and $c = 5.189$ Å [29], and $a = 3.189$ and $c = 5.178$ Å [30] for B4-GaN. The NNP determined shear and bulk moduli for B4-GaN are 93.38 GPa and 204.25 GPa which are in reasonable agreement with the DFT results of 99.42 GPa and 183.44 GPa, respectively. The NNP calculated shear (bulk) moduli of B3-GaN are 85.05 (184.67) GPa, which agree well with the DFT results of 97.79 (183.21) GPa. In addition, the NNP determined relative energy to B4-GaN is 11.56 meV/f.u. for B3-ZnO, which is in excellent agreement with the DFT results of 13.88 meV/f.u..

We carried out short MD simulations of B3-GaN and B4-GaN at various temperatures of 10, 20, 30, 60, 100, 200, 300, 600, 1000, 1500, and 2000 K over 1000 fs with a timestep of 1 fs. The snapshot structures were extracted every 20 MD step, and computed using DFT for validation. Figs. S21a-b present the NNP and DFT predicted energies per atom and atomic forces of a total of 1100 extracted structures, for which the RMSEs of NNP results relative to DFT data are 4.2 meV/atom and 62.4 meV/Å for energies and atomic forces, respectively. Fig. S21c highlights the NNP predicted energies of B4-GaN along the same MD trajectory at 300 K in comparison with their DFT reference, showing that no energy deviates from the DFT references by more than 4.0 meV/atom for B4-GaN at 300 K. Furthermore, as shown in Fig. S21d, the majority of NNP force vectors are within 5° of their DFT references. Our NNP of GaN catches the course of the energy and atomic force well, and we get near DFT accuracy in these simulations using this NNP.

The NNP performance for the phonon dispersion of B3-GaN and B4-GaN compared with the DFT results are shown in Fig. S22. The phonon dispersion curve was calculated via a combination of phonoLAMMPS [12] and PHONOPY [13]. The NNP-predicted phonon dispersion curves of GaN show a reasonable agreement with the DFT results. In addition, the absence of imaginary modes in the whole Brillouin zone confirms these three types of GaN to be dynamically stable.

S3.3 Elastic deformation

Figs. S23a-b illustrate the NNP determined energy of B4-GaN as a function of volumetric strain $\Delta V/V_0$ with or without Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion [14], as well as the DFT results for comparison. The ZBL repulsion only works as $\Delta V/V_0 < -0.45$, which can supply the shortage of NNP as describing the very close atom pairs. Together with the ZBL repulsion, the NNP describes well the deformation of B4-GaN at a wide range of strain $\Delta V/V_0$ from -0.8 to 20.0 . The agreement to DFT results provides

a validation of NNP accuracy. Fig. S23c shows the energy per atom as a function of the cell volume of different GaN polymorphs: wurtzite (B4), Zinc blende (B3), and NaCl (B1), comparing with the DFT reference energies. The results of B1-GaN are also shown for comparison. It is noted that the results of B1-GaN are NOT included in the training data. The NNP results show a good agreement with the DFT results.

S3.4 Cleavage and surface

Fig. S24 shows the NN performance for the binding energy $\chi(d)$ as a function of cleavage opening d without relaxation together with the DFT results for comparison. An agreement is obtained for the binding energy $\chi(d)$ and rigid cleavage energy $\chi_C \equiv \lim_{d \rightarrow \infty} \chi(d)$ of two types of GaN, indicated the successful implementation of our NNP for the cleavage failure of GaN.

Table S8 lists the NNP and DFT predicted surface energy of GaN, which is defined as $(E_s - E_0)/A_s$, where E_s and E_0 are the energies of the surface structure and perfect structure, respectively, and A_s is the area of the surface. The NNP calculated surface energy are 4.14, 1.76, 6.75, 3.31, 6.91, 3.46, 1.84, and 1.77 J/m², which are similar with the DFT results of 4.10, 1.77, 6.32, 3.40, 7.51, 4.34, 2.14, and 1.68 J/m² for the (001), (011), (111) glide-set, and (111) shuffle-set planes of B3-GaN, as well as (0001) glide-set, (0001) shuffle-set, (10 $\bar{1}$ 0) shuffle-set, and (11 $\bar{2}$ 0) planes in B4-GaN, respectively. The surface energy without relaxation, which corresponds to half of the rigid cleavage energy χ_C [15], is also shown in Table S8.

S3.5 Planar defect

The NNP performance for planar defects was also validated. The NNP and DFT predicted formation energy of planar defects shown in Figs. S11 and S12 in GaN defined as $(E_d -$

$E_0)/A_d$ are listed in Table S9, where E_d and E_0 are the energies of the structure consisting of planar defect and the perfect structure, respectively, and A_d is the area of the planar defect. The NNP determined formation energy of planar defects are -0.05 , -0.10 , -0.14 , 0.03 , 0.06 , 0.10 , 0.06 , 0.72 , 0.82 , 9.66 , and 4.33 J/m² for the planar defects of twin, SF, and coherent heterophase interface in B3-GaN, as well as I₁-SF, I₂-SF, I₃-SF, E-SF, IDB-(10 $\bar{1}0$) I, IDB-(11 $\bar{2}0$), IDB-(0001) and IDB-(10 $\bar{1}0$) II planar defects in B4-GaN, which agree well with the DFT results of -0.02 , -0.07 , -0.12 , 0.05 , 0.10 , 0.15 , 0.10 , 0.80 , 0.70 , 10.09 , and 4.35 J/m², respectively.

S3.6 Stacking fault

Fig. S25 shows the NNP performance for the generalized stacking fault energies of B4-GaN compared with the DFT results. The typical slip systems on the basal (0001), prismatic I (10 $\bar{1}0$), prismatic II (11 $\bar{2}0$), pyramidal I (10 $\bar{1}1$), and pyramidal II (11 $\bar{2}2$) planes in the hexagonal close packing (HCP) structure are considered. Especially, in the wurtzite (B4) structure, there include two different slip planes, i.e., glide-set and shuffle-set, on basal (0001) and prismatic I (10 $\bar{1}0$) planes (see Fig. S14). It is noted that the results of pyramidal I and II planes are NOT included in the training data. The NNP predicted generalized stacking fault energy is in good agreement with the DFT results (see Fig. S25), which provides a solid foundation for the simulation of the dislocation-dominant deformation in B4-GaN using this NNP since the stacking fault energy is a fundamental property for the dislocation nucleation and slip [21, 22]. The NNP-determined generalized stacking fault energies of B3-GaN are shown in Fig. S26, which also agree well with the DFT results.

S3.7 Dislocation

The Peierls barriers of the dislocations in B4-GaN are shown in Figs. S16 and S17 calculated via NNP and DFT are shown in Fig. S27, which were determined via the dislocation dipole model of quadrupolar arrangement and the NEB method. To be noted that except the prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, $1/3\langle 11\bar{2}0 \rangle$ screw dislocation, and basal glide-set $1/3\langle 1\bar{1}00 \rangle$ partial screw dislocation, the calculated Peierls barrier of other dislocations is an average value of those with N core and Ga core shown in Figs. S16 and S17. Different simulation cell size was used, which is defined by the number of (n,m) . The NNP results have a great agreement with the DFT results.

Figures

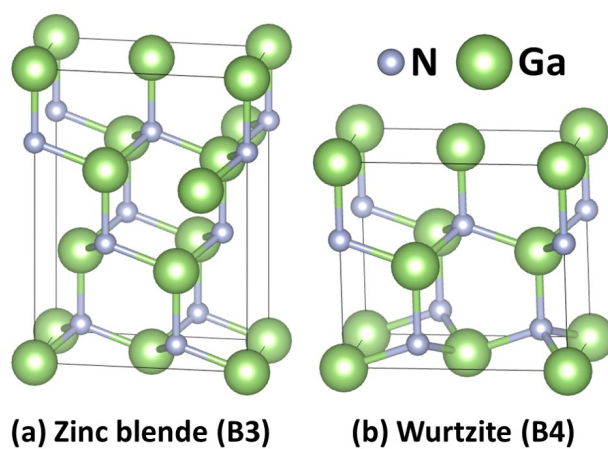


Figure S19: Stick and ball representation of typical GaN polymorphs: (a) cubic zinc blende (B3), and (b) hexagonal wurtzite (B4).

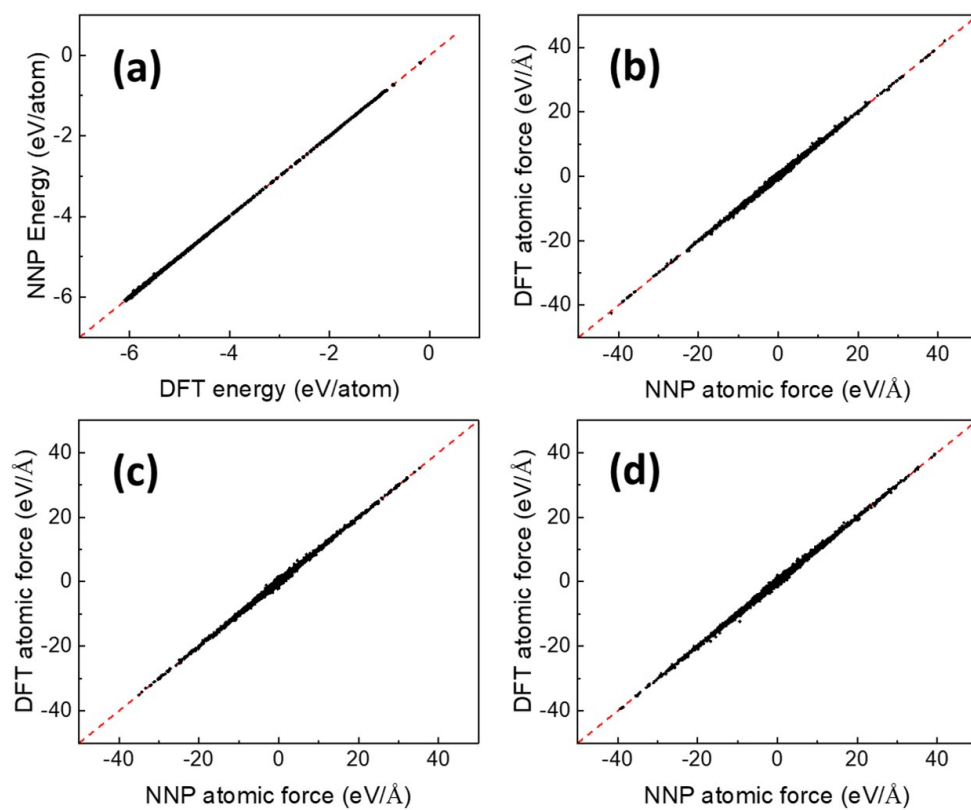


Figure S20: Comparison of DFT and NNP predicted (a) energies and (b-d) components of atomic forces along (b) x -, (c) y - and (d) z -axes of the structures in the training dataset. The line with a slope of 1 corresponds to perfect training.

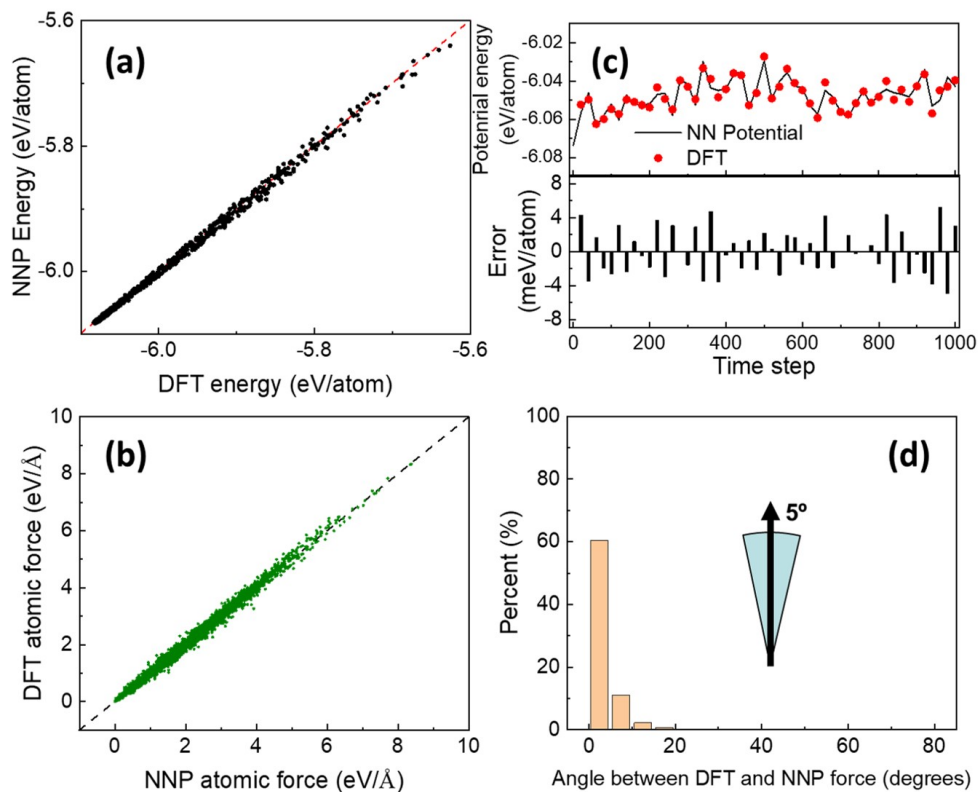


Figure S21: Comparison of the NNP and DFT predicted (a) energies and (b) atomic forces of the extracted structures from a 1000 fs MD trajectory with a time step of 1 fs under different temperatures of 10, 20, 30, 60, 100, 200, 300, 600, 1000, 1500, and 2000 K. The snapshot structures were extracted every 20 MD steps. (c) Energy of B4-GaN predicted by the NNP and DFT calculations along the same MD trajectory at 300 K. (d) Histogram of the absolute directional errors in the NNP prediction of the atomic force. The majority of NNP force vectors are within 5° of their DFT references; this trust region is depicted as the blue area in the inset.

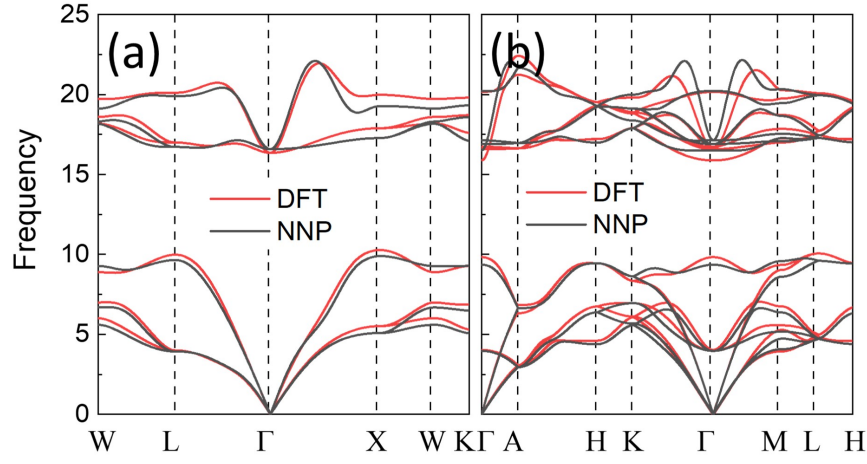


Figure S22: NNP performance for the phonon dispersion of (a) B3-GaN, and (b) B4-GaN, comparing with the DFT results.

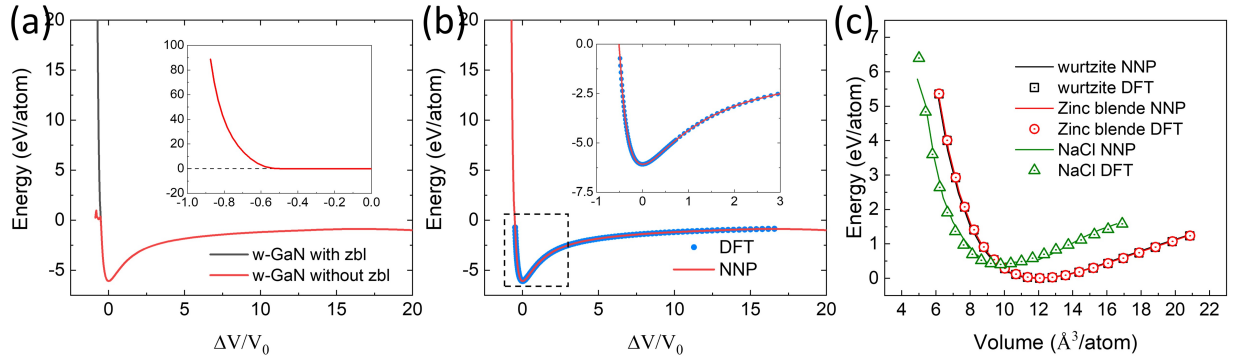


Figure S23: (a-b) The energy of B4-GaN as a function of volumetric strain $\Delta V/V_0$ with or without Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion, as well as the DFT results for comparison. (Insert) The energy resulting from the ZBL repulsion is shown in (a). (c) Energy per atom as a function of the cell volume for the GaN crystal polymorphs: wurtzite (B4), Zinc blende (B3), and NaCl (B1). Symbols correspond to the DFT reference energies and lines interpolate the NNP predicted energies. The results of B1-GaN are also shown for comparison. It is noted that the results of B1-GaN are NOT included in the training dataset.

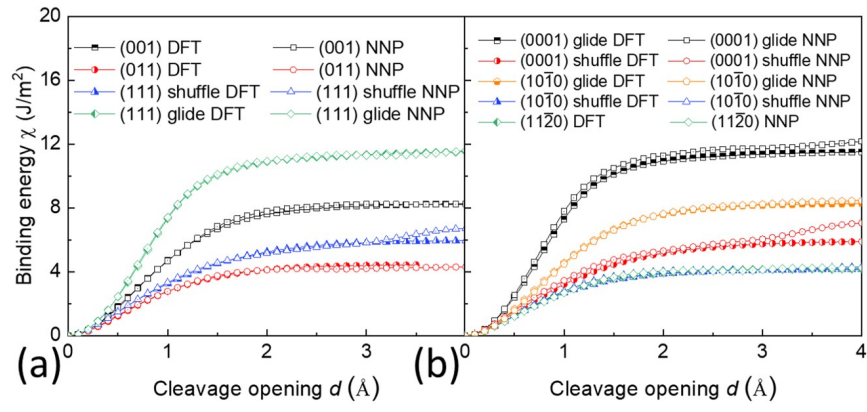


Figure S24: NNP performance for the binding energy curve as a function of cleavage opening d without relaxation: (a) B3-GaN, and (b) B4-GaN, together with the DFT results for comparison.

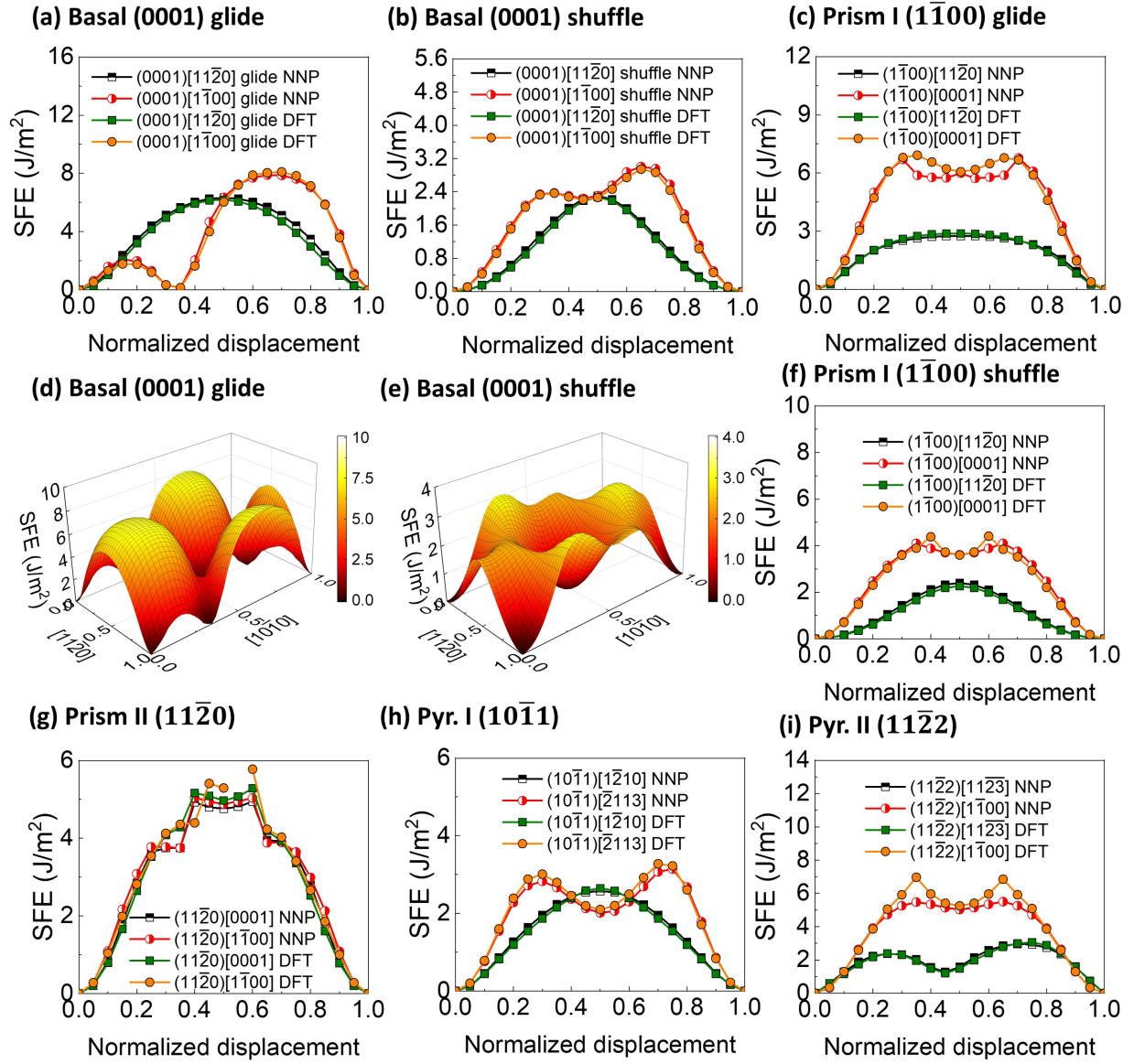


Figure S25: NNP performance for the generalized stacking fault energy of B4-GaN comparing with the DFT results. The orientation of the basal and prismatic I planes of shuffle-set and glide-set are shown in Fig. S14.

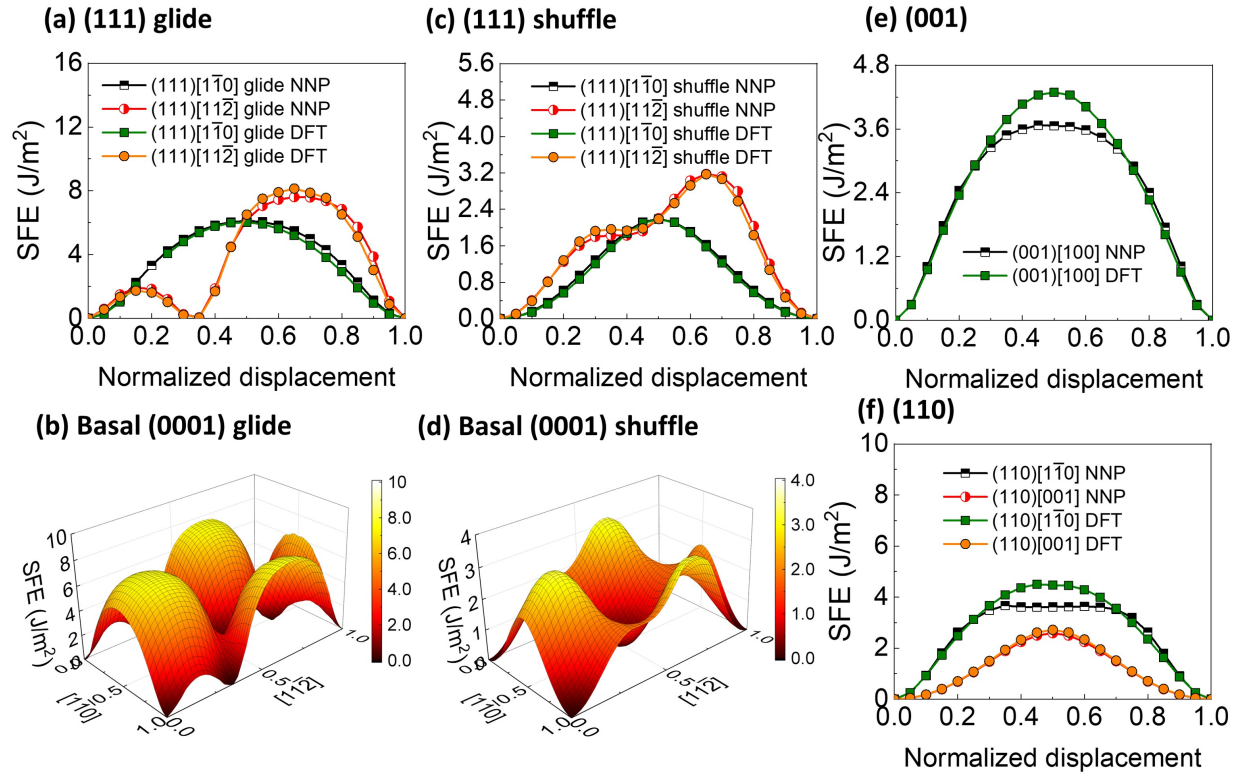


Figure S26: NNP performance for the generalized stacking fault energy of B3-GaN comparing with the DFT results.

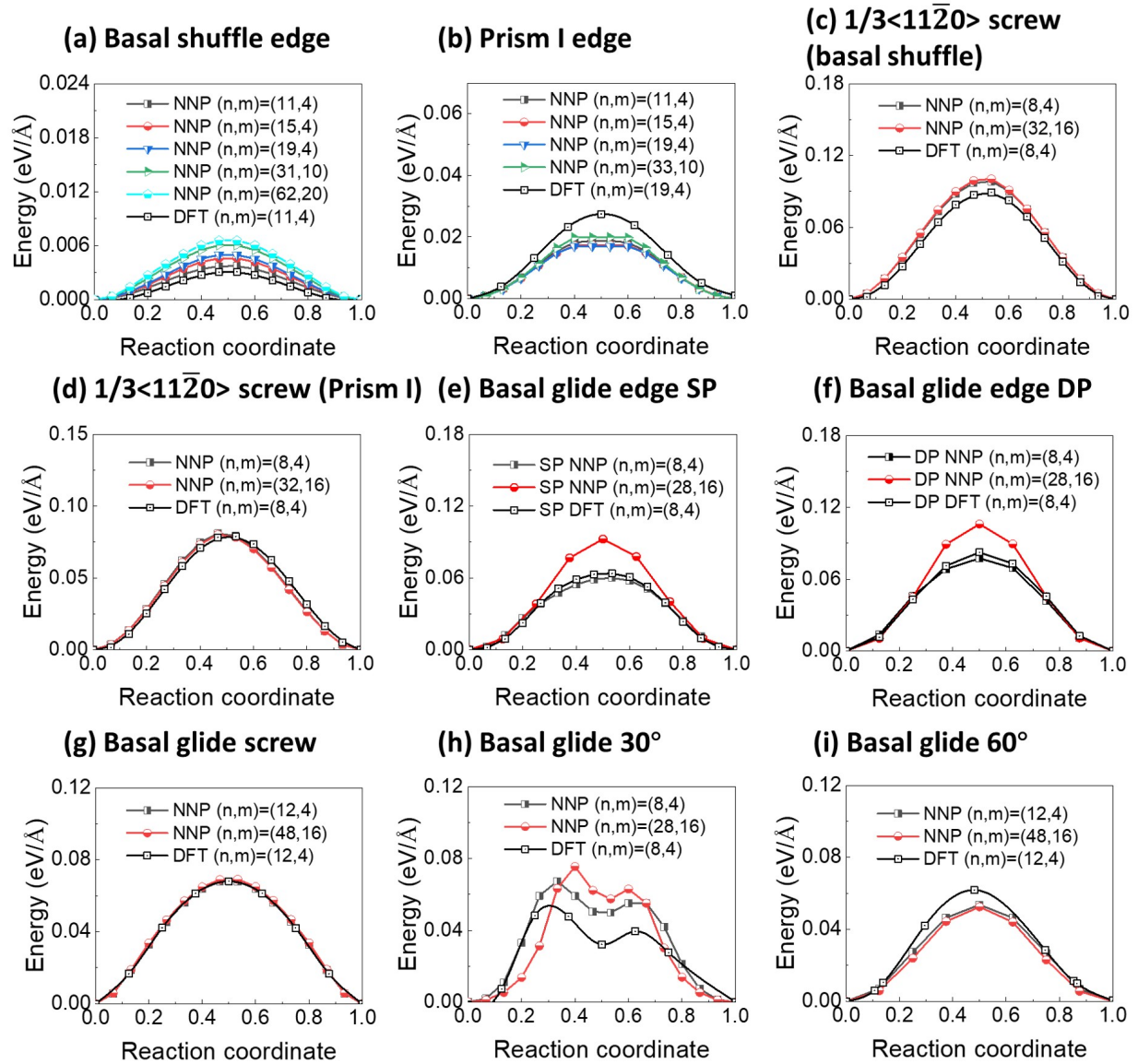


Figure S27: The Peierls barrier of (a) basal shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, (b) prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, $1/3\langle 11\bar{2}0 \rangle$ screw dislocation slipping on (c) basal and (d) prismatic I shuffle-set planes, as well as (e-i) basal glide-set $1/3\langle 1\bar{1}00 \rangle$ partial dislocations slipping on basal glide-set plane. They were calculated via the dislocation dipole model of quadrupolar arrangement and the NEB method. The DFT results are also shown for comparison. To be noted that except the prismatic I shuffle-set $1/3\langle 11\bar{2}0 \rangle$ edge dislocation, $1/3\langle 11\bar{2}0 \rangle$ screw dislocation, and basal glide-set $1/3\langle 1\bar{1}00 \rangle$ partial screw dislocation, the calculated Peierls barrier of other dislocations is an average value of those with N core and Ga core shown in Figs. S16 and S17.

Tables

Table S6: Training dataset employed to construct the NNP of GaN, all of which were calculated via DFT calculations.

Type of str.	Description
Elastic deformation	• The deformation pattern of B3-GaN: $(\varepsilon, 0, 0, 0, 0, 0)$, $(\varepsilon, \varepsilon, 0, 0, 0, 0)$, $(0, 0, 0, \varepsilon, 0, 0)$, $(0, 0, 0, \varepsilon, \varepsilon, 0)$, $(0, 0, 0, \varepsilon, \varepsilon, \varepsilon)$, $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$; • The deformation pattern of B4-GaN: $(\varepsilon, 0, 0, 0, 0, 0)$, $(0, 0, \varepsilon, 0, 0, 0)$, $(\varepsilon, \varepsilon, 0, 0, 0, 0)$, $(\varepsilon, 0, \varepsilon, 0, 0, 0)$, $(0, 0, 0, \varepsilon, 0, 0)$, $(0, 0, 0, 0, 0, \varepsilon)$, $(0, 0, 0, \varepsilon, \varepsilon, 0)$, $(0, 0, 0, \varepsilon, 0, \varepsilon)$, $(0, 0, 0, \varepsilon, \varepsilon, \varepsilon)$, $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$; • The ranges of strain ε are $-0.20 \sim 1.60$ for the $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$ deformation pattern, and $-0.20 \sim 0.20$ for other types of deformation pattern; • Relaxation: No relaxation for both atomic position and cell shape.
Tensile, compress and shear loadings	• Direction of tensile and compress loadings: $[001]$, $[011]$ and $[111]$ for B3-GaN, and $[0001]$, $[11\bar{2}0]$ and $[10\bar{1}0]$ for B4-GaN; • Direction of shear loading: $(001)[100]$, $(001)[110]$, $(110)[001]$, $(110)[1\bar{1}0]$, $(111)[1\bar{1}0]$, $(111)[\bar{1}\bar{1}2]$ and $(111)[11\bar{2}]$ for B3-GaN, and $(0001)[11\bar{2}0]$, $(0001)[10\bar{1}0]$ and $(10\bar{1}0)[0001]$ for B4-GaN; • Strain range: from 0.00 to the strain where the failure occurs; • Relaxation: 1) Full relaxation of both atomic position and cell shape except the applied strain component; 2) No relaxation of both atomic position and cell shape.
Cleavage	• (001), (011) and (111) planes for B3-GaN, and (0001), $(10\bar{1}0)$ and $(11\bar{2}0)$ planes for B4-GaN; • Range of cleavage opening d: $0.0 \sim 4.0$ Å; • Relaxation: No relaxation for both atomic position and cell shape.
Surface	• (001), (011) and (111) planes for B3-GaN, and (0001), $(10\bar{1}0)$ and $(11\bar{2}0)$ planes for B4-GaN; • Thickness of vacuum layer: 15 Å; • Relaxation: 1) Relaxation of the positions of only the atoms whose distance away from surface smaller than 4 Å; 2) No relaxation of both atomic position and cell shape.
Vacancy	• Insert randomly 1 O, 1 Ga, 2 N, 2 Ga, 3 N or 3 Ga vacancies in the supercell structures consisting of 96 atoms for B3-GaN, and 128 atoms for B4-GaN; • Relaxation: 1) Full relaxation of both atomic position and cell shape; 2) No relaxation of both atomic position and cell shape.

Stacking fault	• (001)[010], (001)[100], (011)[100], (011)[01$\bar{1}$], (111)[1$\bar{1}$0] and (111)[11$\bar{2}$] for B3-GaN, and (0001)[10$\bar{1}$0], (0001)[11$\bar{2}$0], (11$\bar{2}$0)[0001], (11$\bar{2}$0)[10$\bar{1}$0], (10$\bar{1}$0)[0001] and (10$\bar{1}$0)[11$\bar{2}$0] for B4-GaN; • Relaxation: 1) Only the atomic movement normal to the slip plane together with cell shape are permitted to relax; 2) No relaxation of both atomic position and cell shape;
Planar defect	• (111) twin, (111) stacking fault, and coherent heterophase interface for B3-GaN; • I1, I2, I3 and extrinsic (E) basal-plane stacking faults, inversion domain boundary of (10$\bar{1}$0), (11$\bar{2}$0) and (0001) planes for B4-GaN; • Relaxation: Full relaxation of both atomic position and cell shape.
Distortion	• Add different random distortions to each atom in the supercell of B3-GaN and B4-GaN to create the distorted structures; • Size of supercell: 1$\times$1$\times$1 unit cell and 2$\times$2$\times$2 supercell for B3-GaN, as well as 2$\times$2$\times$1 and 3$\times$3$\times$2 supercells for B4-GaN; • Atomic coordinate changes from (x, y, z) to $(x + dx, y + dy, z + dz)$, where dx, dy and dz are random values ranging from $-d^{max}$ to d^{max}; • d^{max} (in Å): 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.12, 0.15, 0.20 and 0.25.
Amorphous	• These amorphous structures are created as follows: 1) run 8000 fs with a timestep of 1 fs and a supercell consisting of 96 atoms at 6000 K via VASP AIMD; 2) Full relaxation of both atomic position and lattice constant.
Isolate atom	• The energy of isolate N or Ga atom is calculated; • Size of supercell: 10 Å$\times$10 Å$\times$10 Å, 20 Å$\times$20 Å$\times$20 Å, and 30 Å$\times$30 Å$\times$30 Å.

Table S7: NNP and DFT predicted lattice constant (a and c in Å), elastic constants (c_{ij} in GPa), the polycrystalline shear (μ) and bulk (κ) moduli (in GPa) calculated via the Voigt-Reuss-Hill approximation [7, 8], as well as the relative energy to B4-GaN (ΔE in meV/f.u.). The theoretical values and experimental data previously published in the literature are also shown for comparison.

	a	c	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}	μ	κ	ΔE	Note
B4-GaN	3.224	5.290	335	143	123	392	79	92	93.38	204.25	0.00	This work, NNP
	3.248	5.282	329	128	96	355	86	100	99.42	183.44	0.00	This work, GGA-PBE
	3.190	5.189										Exp. [29]
	3.189	5.178										Exp. [30]
			390	145	106	398	105	123				Exp. [31]
			356	146	115	382	91	105		205		LDA [32]
B3-GaN	4.580		244	155			131		85.05	184.67	11.56	This work, NNP
	4.588		259	145			141		97.79	183.21	13.88	This work, GGA-PBE

Table S8: NNP and DFT predicted surface energy of GaN (in J/m²). Both of the results without relaxation (which corresponds to half of the rigid cleavage energy [15]) and with full relaxation are shown.

	Surface	DFT (unrelaxed)	DFT (fully relaxed)	NNP (unrelaxed)	NNP (fully relaxed)
B3-ZnO	(001)	4.22	4.10	4.37	4.14
	(011)	2.25	1.77	2.37	1.76
	(111) Glide	6.36	6.32	6.96	6.75
	(111) Shuffle	3.58	3.40	3.57	3.31
B4-ZnO	(0001) Glide	7.55	7.51	7.27	6.91
	(0001) Shuffle	4.47	4.34	3.73	3.46
	(10 $\bar{1}$ 0) Glide	-	-	4.44	3.97
	(10 $\bar{1}$ 0) Shuffle	2.62	2.14	2.47	1.84
	(11 $\bar{2}$ 0)	2.10	1.68	2.41	1.77

Table S9: NNP and DFT predicted formation energy of planar defects in GaN (in J/m²). The planar defects include twin, stacking fault (SF) and coherent heterophase interface (CHI) in B3-GaN, as well as the I₁, I₂, I₃ and E types of SF, and the inversion domain boundary (IDB) of (10 $\bar{1}$ 0), (11 $\bar{2}$ 0) and (0001) planes in B4-GaN (see Figs. [S11](#) and [S12](#)).

	Planar defect	DFT	NNP
B3-GaN	Twin	-0.01	-0.03
	SF	-0.04	-0.05
	CHI	-0.06	-0.07
B4-GaN	I ₁ -SF	0.02	0.01
	I ₂ -SF	0.05	0.03
	I ₃ -SF	0.07	0.05
	E-SF	0.05	0.03
	IDB-(10 $\bar{1}$ 0) I	0.40	0.36
	IDB-(11 $\bar{2}$ 0)	0.35	0.41
	IDB-(0001)	5.05	4.83
	IDB-(10 $\bar{1}$ 0) II	2.17	2.17

S4 Neural network potential of SrTiO₃

S4.1 Detail of training dataset

The detail of the training dataset for the SrTiO₃ NNP is shown in Table S10. Two typical SrTiO₃ polymorphs were considered, including cubic (Pm $\bar{3}$ m) and tetragonal (I4/mcm) phases (see Fig. S28).

S4.2 Equilibrium structure

Fig. S29 shows the comparison of DFT and NNP predicted energies and components of atomic forces along x -, y - and z -axes of the structures in the training dataset. The root mean square errors (RMSEs) of SrTiO₃ NNP for energy and atomic force are 2.5 meV/atom and 89.6 meV/Å, respectively.

As shown in Table S11, we firstly compared the NNP and DFT predicted lattice constants, elastic constants, polycrystalline bulk and shear moduli, as well as the relative energy to c-SrTiO₃. The elastic constants of SrTiO₃ were determined via the AELAS code [6], and the polycrystalline bulk and shear moduli were calculated using the Voigt-Reuss-Hill approximation [7, 8]. The NNP predicted lattice constants are $a = 3.896$ Å of c-SrTiO₃, and $a = 5.500$ and $c = 7.832$ Å of t-SrTiO₃, which are very close to the DFT predicted value of 3.895, 5.494, and 7.815 Å in this work, as well as 3.895, 5.494, and 7.812 Å in Ref. [33], respectively. The NNP determined shear and bulk moduli for c-SrTiO₃ are 109.20 GPa and 189.00 GPa which are in reasonable agreement with the DFT results of 118.03 GPa and 186.04 GPa, respectively. The NNP calculated shear (bulk) moduli of t-SrTiO₃ are 86.99 (181.57) GPa, which agree well with the DFT results of 105.97 (182.99) GPa, respectively. In addition, the NNP determined relative energy to t-SrTiO₃ is -8.80 meV/f.u. for t-SrTiO₃, which is in excellent agreement with the DFT results of -5.72 meV/f.u..

We carried out short MD simulations of c-SrTiO₃ and t-SrTiO₃ at various temperatures

of 10, 20, 30, 60, 100, 200, 300, 600, 1000, 1500, and 2000 K over 1000 fs with a timestep of 1 fs. The snapshot structures were extracted every 20 MD step, and computed using DFT for validation. Figs. S30a-b present the NNP and DFT predicted energies and atomic forces of a total of 1100 extracted structures, for which the RMSEs of NNP results relative to DFT data are 2.2 meV/atom and 75.2 meV/Å for energies and atomic forces, respectively. Fig. S30c highlights the NNP predicted energies of c-SrTiO₃ along the same MD trajectory at 300 K in comparison with their DFT reference, showing that no energy deviates from the DFT references by more than 2.0 meV/atom for c-SrTiO₃ at 300 K. Furthermore, as shown in Fig. S30d, the majority of NNP force vectors are within 5° of their DFT references. Our NNP of SrTiO₃ catches the course of the energy and atomic force well, and we get near DFT accuracy in these simulations using this NNP.

The NNP performance for the phonon dispersion of c-SrTiO₃ and t-SrTiO₃ compared with the DFT results are shown in Fig. S31. The phonon dispersion curve was calculated via a combination of phonoLAMMPS [12] and PHONOPY [13]. The NNP-predicted phonon dispersion curves of SrTiO₃ show a reasonable agreement with the DFT results.

S4.3 Elastic deformation

Figs. S32a-b illustrate the NNP determined energy of c-SrTiO₃ as a function of volumetric strain $\Delta V/V_0$ with or without Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion [14], as well as the DFT results for comparison. The ZBL repulsion only works as $\Delta V/V_0 < -0.45$, which can supply the shortage of NNP as describing the very close atom pairs. Together with the ZBL repulsion, the NNP describes well the deformation of c-SrTiO₃ at a wide range of strain $\Delta V/V_0$ from -0.8 to 20.0 . The agreement to DFT results provides a validation of NNP accuracy. Fig. S32c shows the energy per atom as a function of the cell volume of c-SrTiO₃ and t-SrTiO₃ polymorphs, compared with the DFT reference energies. The NNP results show a good agreement with the DFT results.

S4.4 Cleavage and surface

Fig. S33 shows the NN performance for the binding energy $\chi(d)$ as a function of cleavage opening d without relaxation together with the DFT results for comparison. An agreement is obtained for the binding energy $\chi(d)$ and rigid cleavage energy $\chi_C \equiv \lim_{d \rightarrow \infty} \chi(d)$ of two types of SrTiO₃, indicated the successful implementation of our NNP for the cleavage failure of SrTiO₃.

Table S12 lists the NNP and DFT predicted surface energy of SrTiO₃, which is defined as $(E_s - E_0)/A_s$, where E_s and E_0 are the energies of the surface structure and perfect structure, respectively, and A_s is the area of the surface. The NNP calculated surface energy are 1.10, 1.06, 1.07, and 1.08 J/m², which are similar to the DFT results 1.12, 1.09, 1.05, and 1.09 J/m² for the (001) plane of c-SrTiO₃, as well as (001), (100), and (110) planes in t-SrTiO₃, respectively. The surface energy without relaxation, which corresponds to half of the rigid cleavage energy χ_C [15], is also shown in Table S12.

S4.5 Stacking fault

Fig. S34 shows the NNP performance for the generalized stacking fault energies of c-SrTiO₃ compared with the DFT results. The typical slip systems on the (001), (011), (111), and (112) planes in the cubic structure are considered. The NNP predicted generalized stacking fault energy is in good agreement with the DFT results (see Fig. S34), which provides a solid foundation for the simulation of the dislocation-dominant deformation in c-SrTiO₃ using this NNP since the stacking fault energy is a fundamental property for the dislocation nucleation and slip [21, 22]. The NNP-determined generalized stacking fault energies of t-SrTiO₃ are shown in Fig. S35, which also agree well with the DFT results.

S4.6 Dislocation

For the performance of SrTiO₃ NNP for dislocation, five types of dislocation were checked, including $1/2\langle 110 \rangle$ edge dislocation with a $\langle 001 \rangle$ line vector and a $\{1\bar{1}0\}$ slip plane (Fig. S36), $1/2\langle 110 \rangle$ screw dislocation (Fig. S37), $\langle 110 \rangle$ mixed dislocation with a $\langle 100 \rangle$ line vector and a $\{001\}$ slip plane (Fig. S38), $\langle 001 \rangle$ edge dislocation with a $\langle 1\bar{1}0 \rangle$ line vector and a $\{110\}$ slip plane (Fig. S39 and Fig. 9 in the main text), as well as $\langle 110 \rangle$ mixed dislocation with a $\langle 111 \rangle$ line vector and a $\{1\bar{1}0\}$ slip plane (Fig. 10 in the main text). The as-created dislocation configurations were carefully relaxed. By step-wise removal of constraints to the atomic movement, we avoided the unphysical reconstruction of the dislocation cores. The energy of the configurations was measured during NPT molecular dynamics runs at temperatures of 50 K and zero applied pressure. Each dislocation configuration was simulated multiple times with different temperature initializations of the MD simulation to check for consistency.

The equilibrium structures of these dislocations after relaxation via NNP are shown in Figs. S36-S39. These structures relaxed via pair empirical potential [34] are also shown for comparison. For the $1/2\langle 110 \rangle$ edge dislocation with a $\langle 001 \rangle$ line vector and a $\{1\bar{1}0\}$ slip plane, an equilibrium climb splitting of three unit cells (i.e., $3a[1\bar{1}0]$ and 16.5 Å) is evident, which corresponds well to the value of 20 Å observed experimentally [1]. A growing stacking fault and decreasing elastic interactions increase energy at high climb-splitting distances. Similar results were obtained via NNP and pair empirical potential. However, the energy difference between the dislocation dipole models with and without charge balance determined via pair potential is much larger than that obtained via NNP, which results from the electrostatic interaction between the charged dislocation core and each atom with fixed charge in pair empirical potential. The distance of the glide dissociation of $1/2\langle 110 \rangle$ screw dislocation is about 24.9 Å as shown in Fig. S38a, with the stable SFE (850 mJ/m²)

predicted by NNP and DFT. In comparison, due to the larger stable SFE of 1280 mJ/m^2 predicted by the pair empirical potential [34], the splitting distance is $16.7 \text{ \AA}$ (see Fig. S38b).

Figures

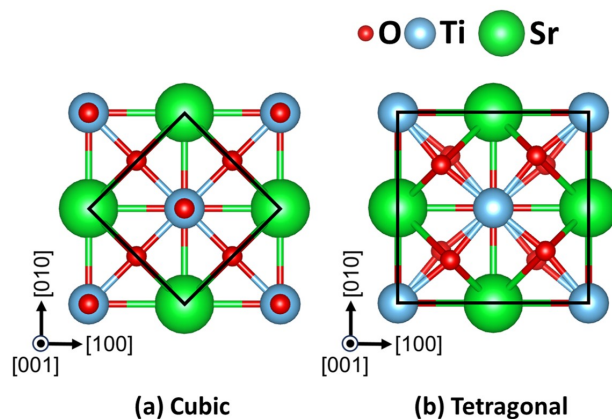


Figure S28: Stick and ball representation of typical SrTiO_3 polymorphs: (a) cubic (c) SrTiO_3 , (b) tetragonal (t) SrTiO_3 .

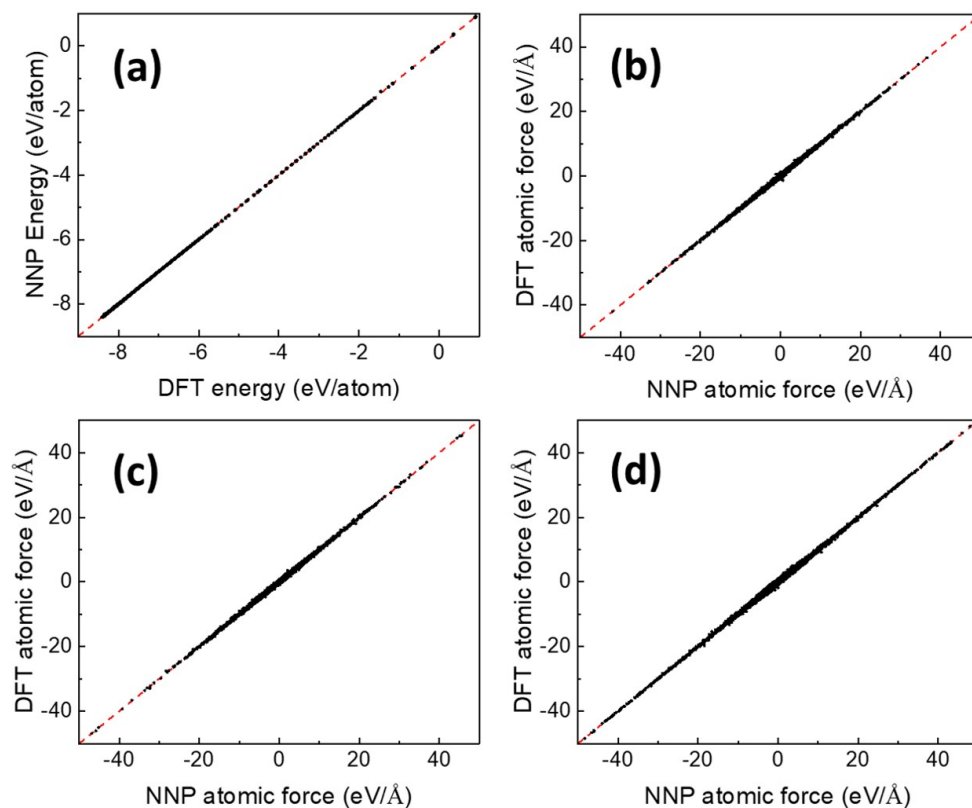


Figure S29: Comparison of DFT and NNP predicted (a) energies and (b-d) components of atomic forces along (b) x -, (c) y - and (d) z -axes of the structures in the training dataset. The line with a slope of 1 corresponds to perfect training.

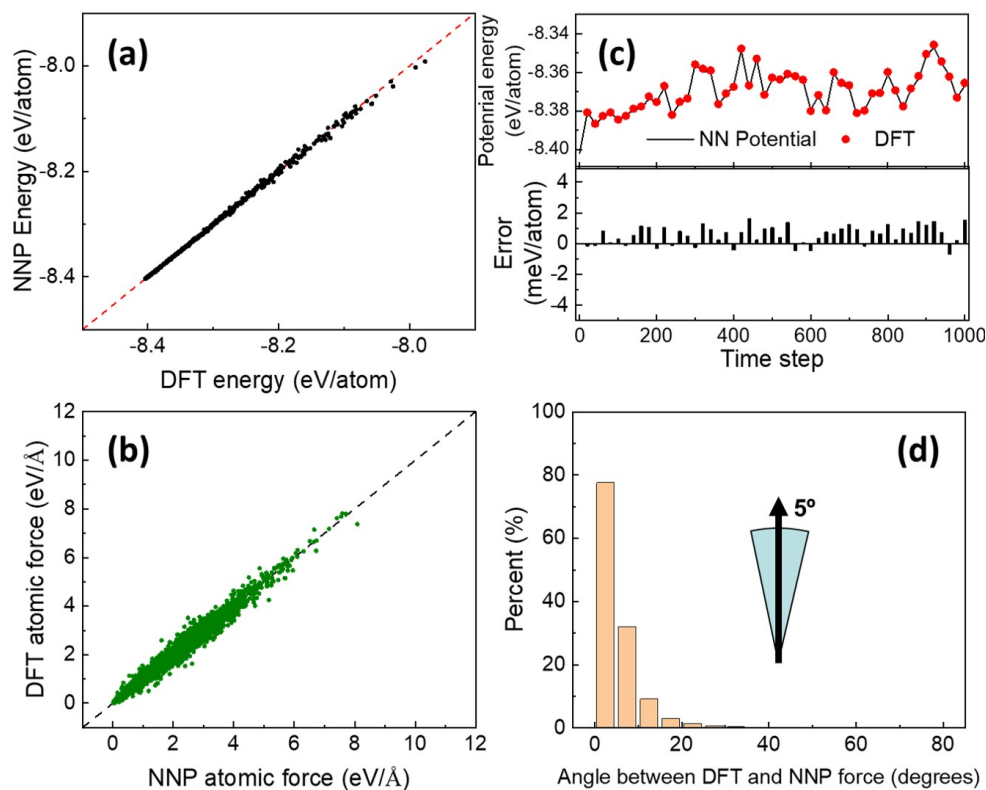


Figure S30: Comparison of the NNP and DFT predicted (a) energies and (b) atomic forces of the extracted structures from a 1000 fs MD trajectory with a time step of 1 fs under different temperatures of 10, 20, 30, 60, 100, 200, 300, 600, 1000, 1500, and 2000 K. The snapshot structures were extracted every 20 MD steps. (c) Energy of c-SrTiO₃ predicted by the NNP and DFT calculations along the same MD trajectory at 300 K. (d) Histogram of the absolute directional errors in the NNP prediction of the atomic force. The majority of NNP force vectors are within 5° of their DFT references; this trust region is depicted as the blue area in the inset.

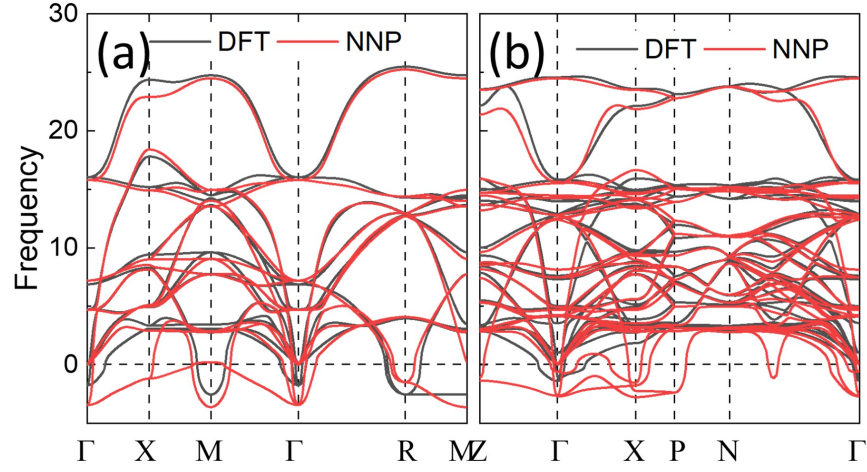


Figure S31: NNP performance for the phonon dispersion of (a) c-SrTiO₃, and (b) t-SrTiO₃, comparing with the DFT results.

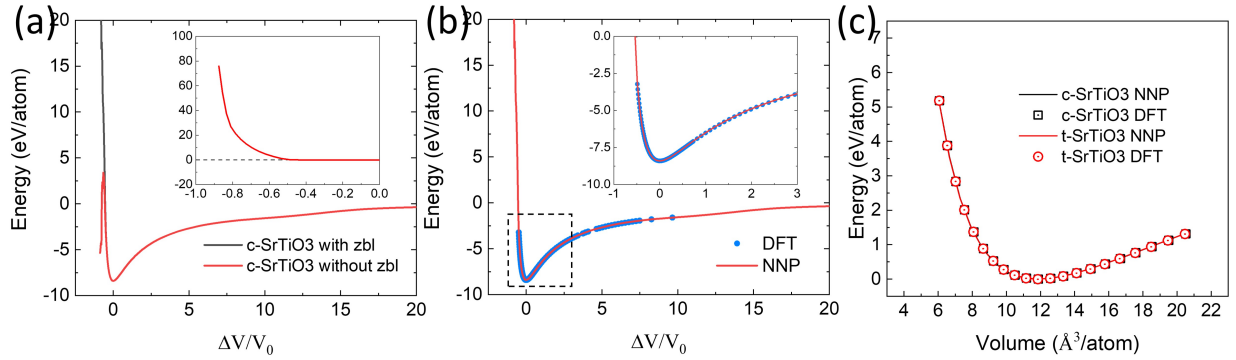


Figure S32: (a-b) The energy of c-SrTiO₃ as a function of volumetric strain $\Delta V/V_0$ with or without Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion, as well as the DFT results for comparison. (Insert) The energy resulting from the ZBL repulsion is shown in (a). (c) Energy per atom as a function of the cell volume for c-SrTiO₃ and t-SrTiO₃. Symbols correspond to the DFT reference energies and lines interpolate the NNP predicted energies.

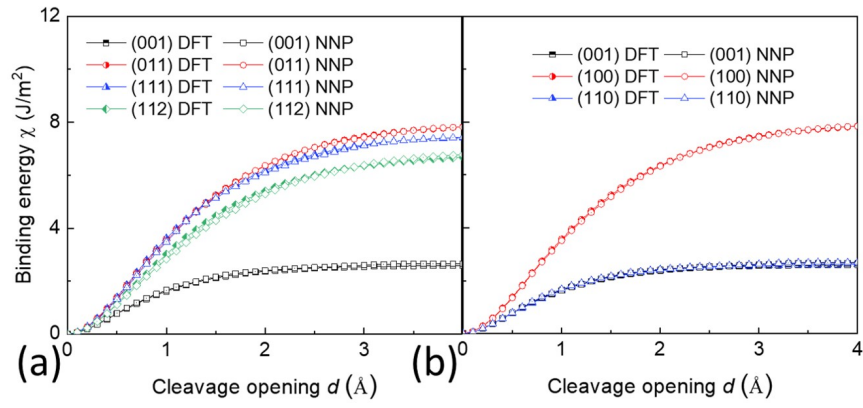


Figure S33: NNP performance for the binding energy curve as a function of cleavage opening d without relaxation: (a) c-SrTiO₃, and (b) t-SrTiO₃, together with the DFT results for comparison.

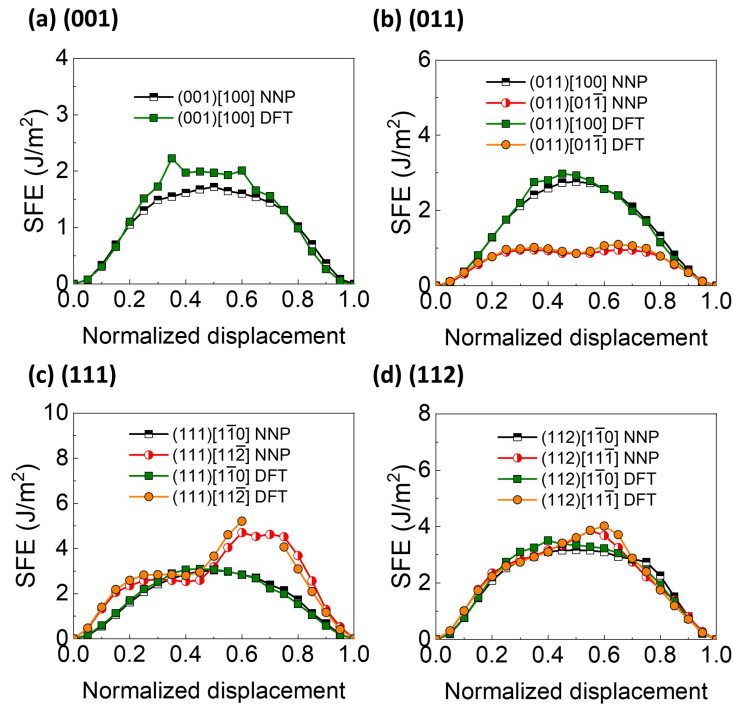


Figure S34: NNP performance for the generalized stacking fault energy of c-SrTiO₃ comparing with the DFT results.

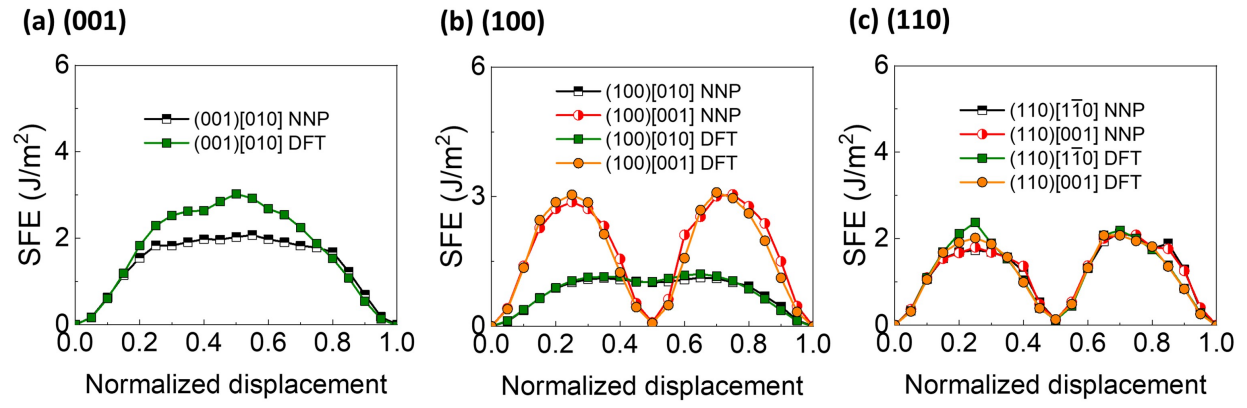


Figure S35: NNP performance for the generalized stacking fault energy of $t\text{-SrTiO}_3$ comparing with the DFT results.

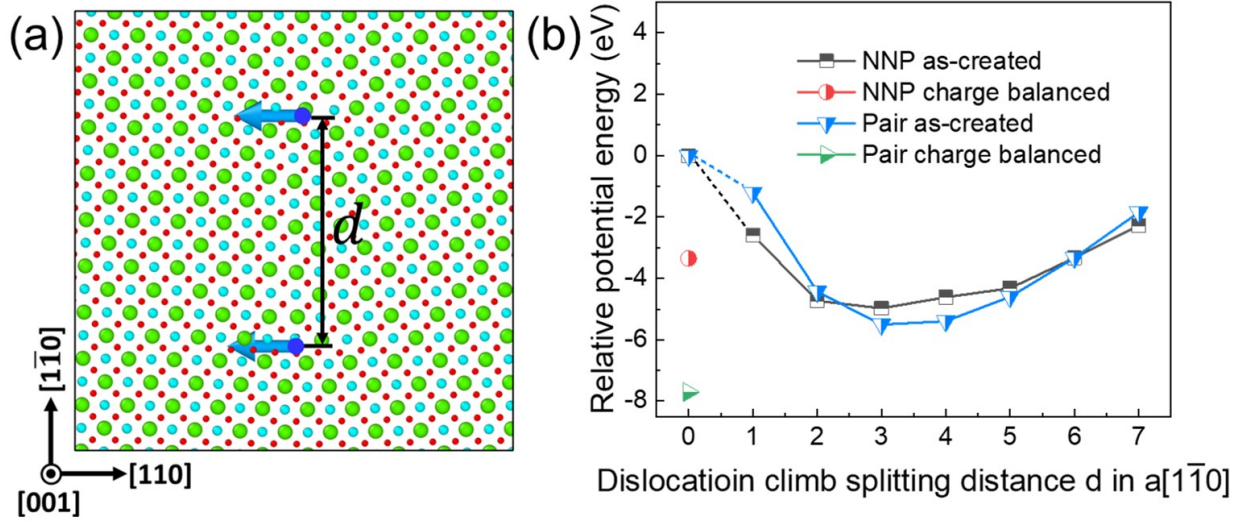


Figure S36: (a) The $1/2\langle 110 \rangle$ edge dislocation with a line vector $\langle 001 \rangle$ and a $\{1\bar{1}0\}$ slip plane in its climb dissociated form cut from a larger sample. The dislocation lines are highlighted by blue lines, and the Burgers vector is shown by the cyan arrows, which were determined based on the Sr-O FCC sublattice via dislocation extraction algorithm (DXA) [4]. (b) The relative potential energy of the dipole models as a function of the climb splitting distances defined in (a). The as-created dislocation is not charge-balanced. The results of the charge-balanced dislocation are also shown for comparison, which is realized by moving one oxygen ion per unit cell dislocation line length from the layer of oxygen ions at the negative code to the positive code before dislocation relaxation [35].

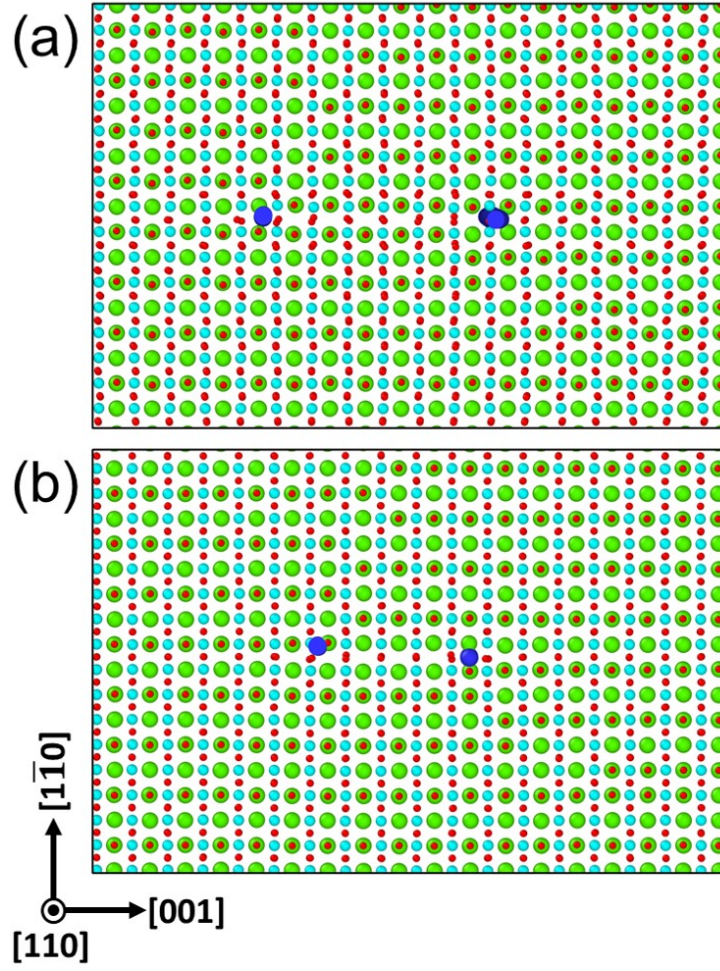


Figure S37: The equilibrium structure of $1/2\langle 110 \rangle$ screw dislocation in its glide dissociated form cut from a larger sample after relaxed via (a) NNP and (b) pair empirical potential [34]. The location of partial dislocations determined based on the Sr-O FCC sublattice via dislocation extraction algorithm (DXA) [4] is highlighted by bulk line.

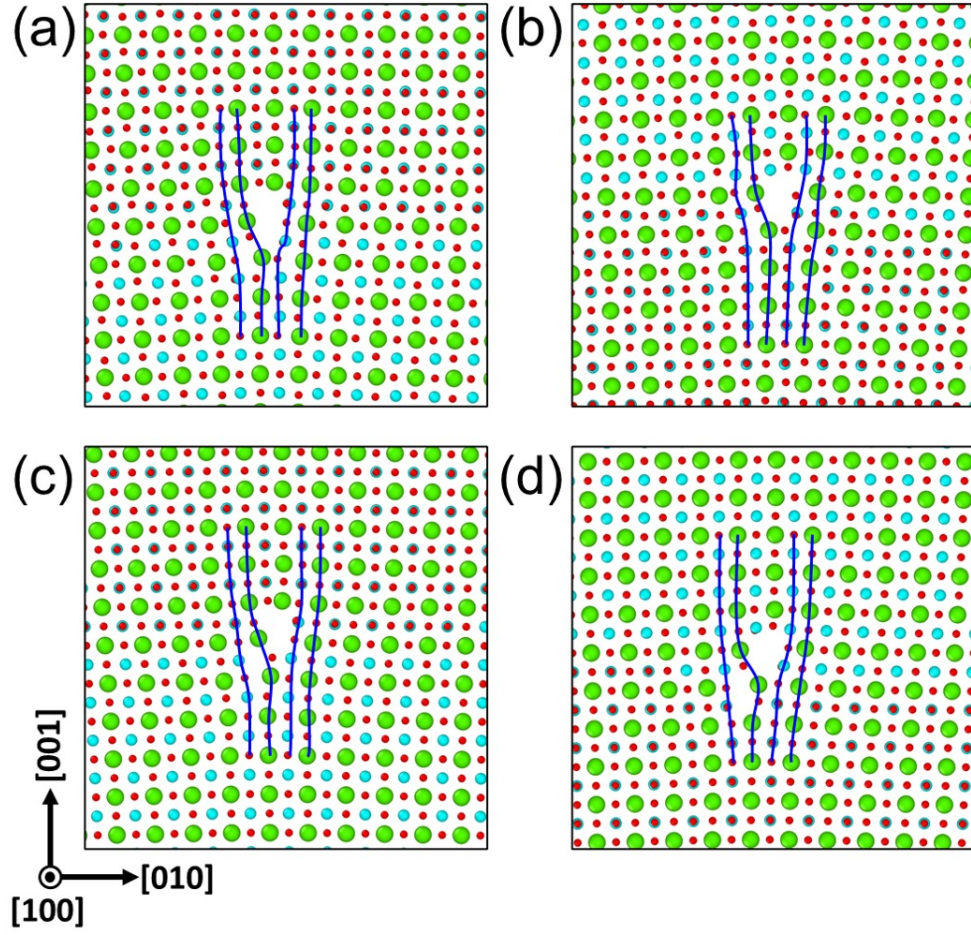


Figure S38: The equilibrium structure of the dislocation being of mixed type $\mathbf{b} = \langle 110 \rangle$ but a $\langle 100 \rangle$ line vector and a $\{001\}$ slip plane cut from a larger sample after relaxed via (a-b) NNP and (c-d) pair empirical potential [34]. Both of the dislocations with (a,c) SrO terminal layer and (b,d) TiO₂ terminal layer are shown. It is noted that both the cores of the SrO and TiO₂ terminated dislocations are charged.

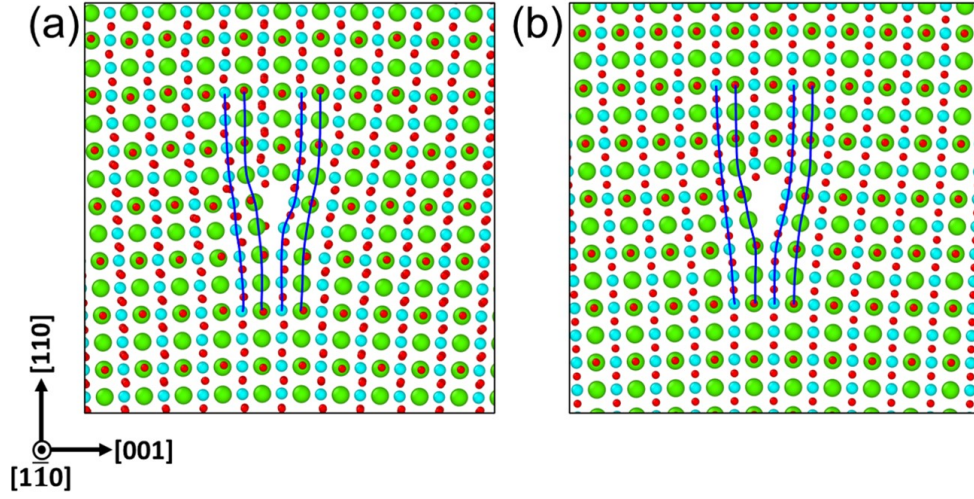


Figure S39: The equilibrium structure of charge-balanced $\langle 001 \rangle$ edge dislocation with a line vector $\langle 110 \rangle$ and a $\{110\}$ slip plane cut from a larger sample after relaxed via (a) NNP and (b) pair empirical potential [34]. For the charge-balanced dislocation core, one of two extra oxygen atoms along the $[1\bar{1}0]$ column was moved from the negatively charged dislocation core to the positively charged dislocation core as shown in Fig. 9.

Tables

Table S10: Training dataset employed to construct the NNP of SrTiO₃, all of which were calculated via DFT calculations.

Type of str.	Description
Elastic deformation	• The deformation pattern of c-SrTiO₃: $(\varepsilon, 0, 0, 0, 0, 0)$, $(\varepsilon, \varepsilon, 0, 0, 0, 0)$, $(0, 0, 0, \varepsilon, 0, 0)$, $(0, 0, 0, \varepsilon, \varepsilon, 0)$, $(0, 0, 0, \varepsilon, \varepsilon, \varepsilon)$, $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$; • The deformation pattern of t-SrTiO₃: $(\varepsilon, 0, 0, 0, 0, 0)$, $(0, 0, \varepsilon, 0, 0, 0)$, $(\varepsilon, \varepsilon, 0, 0, 0, 0)$, $(\varepsilon, 0, \varepsilon, 0, 0, 0)$, $(0, 0, 0, \varepsilon, 0, 0)$, $(0, 0, 0, 0, 0, \varepsilon)$, $(0, 0, 0, \varepsilon, \varepsilon, 0)$, $(0, 0, 0, \varepsilon, 0, \varepsilon)$, $(0, 0, 0, \varepsilon, \varepsilon, \varepsilon)$, $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$; • The ranges of strain ε are $-0.20 \sim -0.06$ and $0.06 \sim 1.60$ for the $(\varepsilon, \varepsilon, \varepsilon, 0, 0, 0)$ deformation pattern, and $-0.20 \sim -0.06$ and $0.06 \sim 0.20$ for other types of deformation pattern; • Relaxation: No relaxation for both atomic position and cell shape.
Tensile, compress and shear loadings	• Direction of tensile and compress loadings: $[001]$, $[011]$ and $[111]$ for c-SrTiO₃, and $[001]$, $[011]$, $[100]$, $[110]$ and $[111]$ for t-SrTiO₃; • Direction of shear loading: $(001)[010]$, $(001)[110]$, $(110)[1\bar{1}0]$, $(111)[1\bar{1}0]$, $(111)[\bar{1}\bar{1}2]$, and $(111)[11\bar{2}]$ for c-SrTiO₃, and $(001)[100]$, $(001)[110]$, $(100)[010]$, $(100)[011]$, $(101)[10\bar{1}]$, and $(110)[1\bar{1}0]$ for t-SrTiO₃; • Strain range: from 0.00 to the strain where the failure occurs; • Relaxation: 1) Full relaxation of both atomic position and cell shape except the applied strain component; 2) No relaxation of both atomic position and cell shape.
Cleavage	• (001), (011), (111), and (112) planes for c-SrTiO₃, and (001), (100), and (110) planes for t-SrTiO₃; • Range of cleavage opening d: $0.0 \sim 4.0$ Å; • Relaxation: No relaxation for both atomic position and cell shape.
Surface	• (001), (011), (111), and (112) planes for c-SrTiO₃, and (001), (100), and (110) planes for t-SrTiO₃; • Thickness of vacuum layer: 15 Å; • Relaxation: 1) Relaxation of the positions of only the atoms whose distance away from surface smaller than 4 Å; 2) No relaxation of both atomic position and cell shape.

Vacancy	• Insert randomly 1 Sr, 1 Ti, 1 O, 2 Sr, 2 Ti, 2 O, 3 Sr, 3 Ti, or 3 O vacancies in the supercell structures consisting of 135 atoms for c-SrTiO₃, and 160 atoms for t-SrTiO₃; • Relaxation: 1) Full relaxation of both atomic position and cell shape; 2) No relaxation of both atomic position and cell shape.
Stacking fault	• (001)[010], (011)[100], (011)[01$\bar{1}$], (111)[1$\bar{1}$0], (111)[11$\bar{2}$], (112)[1$\bar{1}$0], (112)[11$\bar{1}$], (410)[001], and (410)[4$\bar{1}$0] for c-SrTiO₃, and (001)[010], (100)[010], (100)[001], (110)[001], and (110)[1$\bar{1}$0] for t-SrTiO₃; • Relaxation: 1) Only the atomic movement normal to the slip plane together with cell shape are permitted to relax; 2) No relaxation of both atomic position and cell shape;
Isolate atom	• The energy of isolate Sr, Ti or O atom is calculated; • Size of supercell: 10 Å×10 Å×10 Å, 20 Å×20 Å×20 Å, and 30 Å×30 Å×30 Å.

Table S11: NNP and DFT predicted lattice constant (a and c in Å), elastic constants (c_{ij} in GPa), the polycrystalline shear (μ) and bulk (κ) moduli (in GPa) calculated via the Voigt-Reuss-Hill approximation [7, 8], as well as the relative energy to c-SrTiO₃ (ΔE in meV/f.u.). The theoretical values and experimental data previously published in the literature are also shown for comparison.

	a	c	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}	μ	κ	ΔE	Note
c-SrTiO ₃	3.896		333	117			110		109.20	189.00	0.00	This work, NNP
	3.895		351	103			114		118.03	186.04	0.00	This work, GGA-PBEsol
			317.2	102.5			122.35					Exp. [36]
			319.3	97.5			113					GGA-PBE [37]
			290.7	93.9			110.9					BLYP [37]
	3.895		352	105			116					GGA-PBEsol [33]
tetragonal SrTiO ₃	5.500	7.832	318	111	123	285	70	116	86.99	181.57	-8.80	This work, NNP
	5.494	7.815	320	95	97	343	120	121	105.97	182.99	-5.72	This work, GGA-PBEsol
	5.494	7.812	352	103	108	357	116	116				GGA-PBEsol [33]

Table S12: NNP and DFT predicted surface energy of SrTiO_3 (in J/m^2). Both of the results without relaxation (which corresponds to half of the rigid cleavage energy [15]) and with full relaxation are shown.

	Surface	DFT (unrelaxed)	DFT (fully relaxed)	NNP (unrelaxed)	NNP (fully relaxed)
c- SrTiO_3	(001)	1.33	1.12	1.34	1.10
	(011)	4.14	-	3.94	2.64
	(111)	3.76	-	3.76	2.78
	(112)	3.45	-	3.45	2.38
t- SrTiO_3	(001)	1.29	1.09	1.30	1.06
	(100)	1.78	1.05	1.84	1.07
	(110)	1.29	1.09	1.31	1.08

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