Supporting information (SI)

Monitoring the Melting Behavior of Boron Nanoparticles by a Neural Network Potential

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In the supplementary material, we present:

- Figure S1. Electron localization function (ELF) profiles and isosurfaces of α-Boron and α-B_2O_3. The isosurfaces correspond to the value of 0.8.
- Figure S2. Global Lindemann index evolutions for particles with a diameter in 3 nm and corresponding variations with different heating rate.
- Figure S3. Simulation walltime for particles with different diameter at a heating rate in 0.27 K/ps. The total simulation time corresponds to 10 ns.
- Figure S4. Mean absolute error of system energy and atomic force for ReaxFF models on the DFT database.
- Figure S5. Equation of state curve for α-boron and α-B_2O_3 crystals.
- Figure S6. Projected coordinates for boron and oxygen atoms in α-B_2O_3 obtained from ReaxFF simulations with a timestep in 2 fs.
- Figure S7. Computational cost of NNP-GPU (red square), NNP-CPU (purple square) and ReaxFF-CPU (blue square) methods on bulk α-B_2O_3 systems with 135 to 131820 atoms.

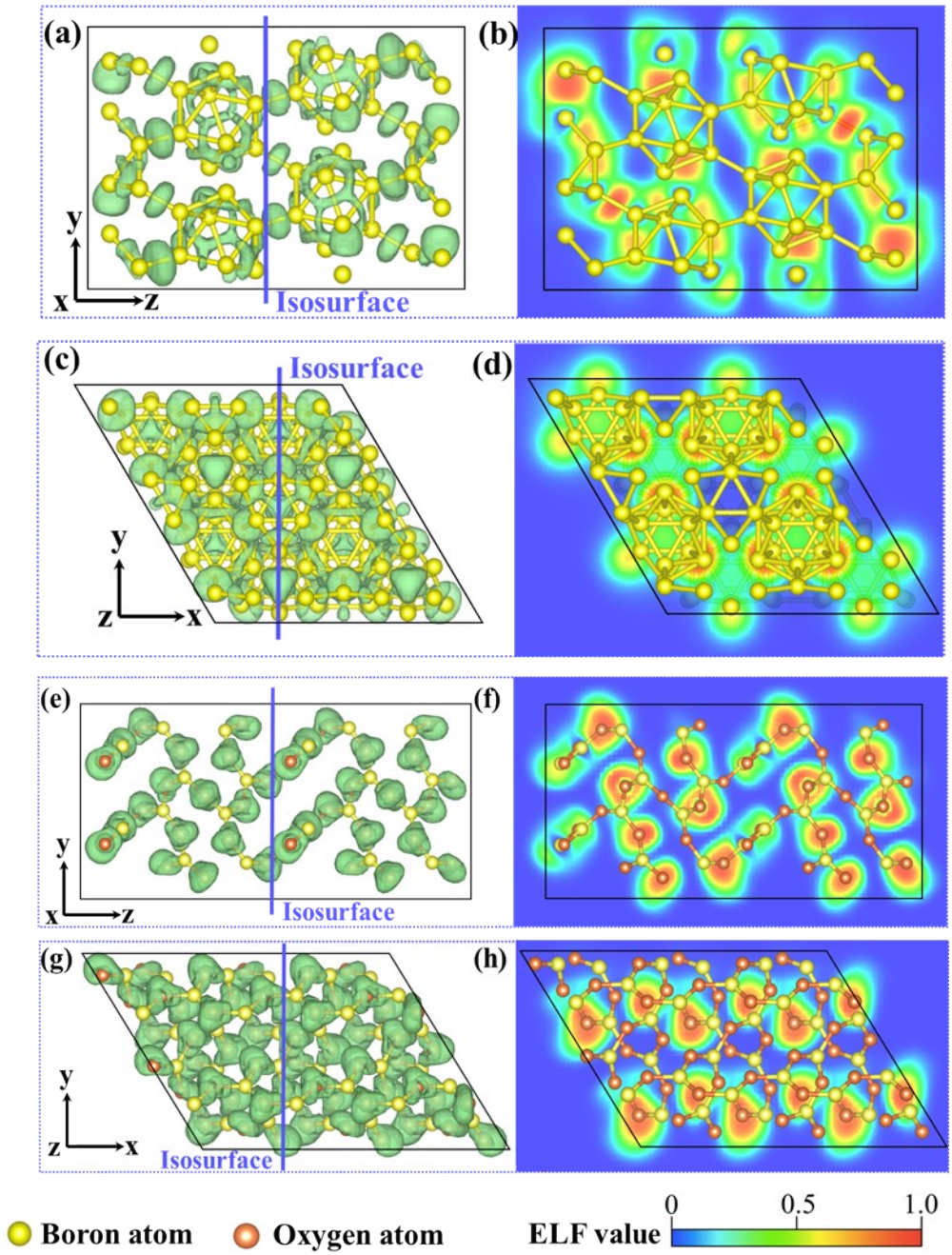

Figure S1. Figure S1. Electron localization function (ELF) profiles and isosurfaces of α-Boron (a-d) and α-B_2O_3 (e-h). The isosurfaces correspond to the value of 0.8.

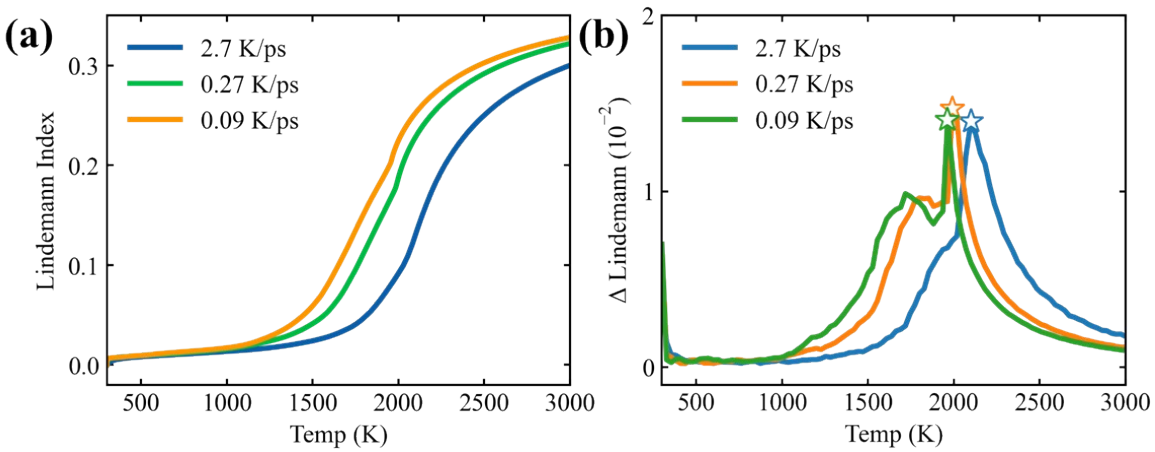

Figure S2. (a) Global Lindemann index evolutions for particles with a diameter in 3 nm and (b) the corresponding variations with heating rate.

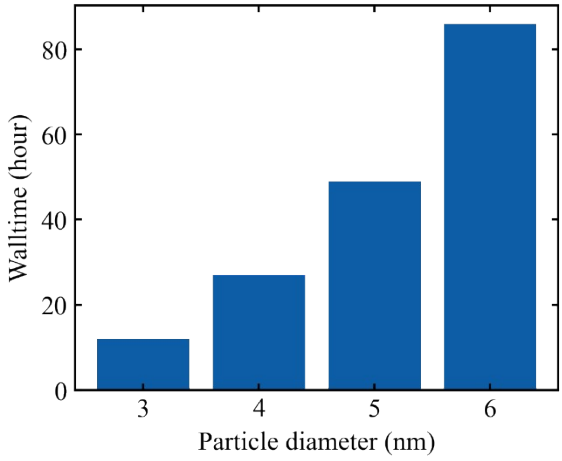

Figure S3. Simulation walltimes for particles with different diameter at a heating rate in 0.27 K/ps. The total simulation time corresponds to 10 ns.

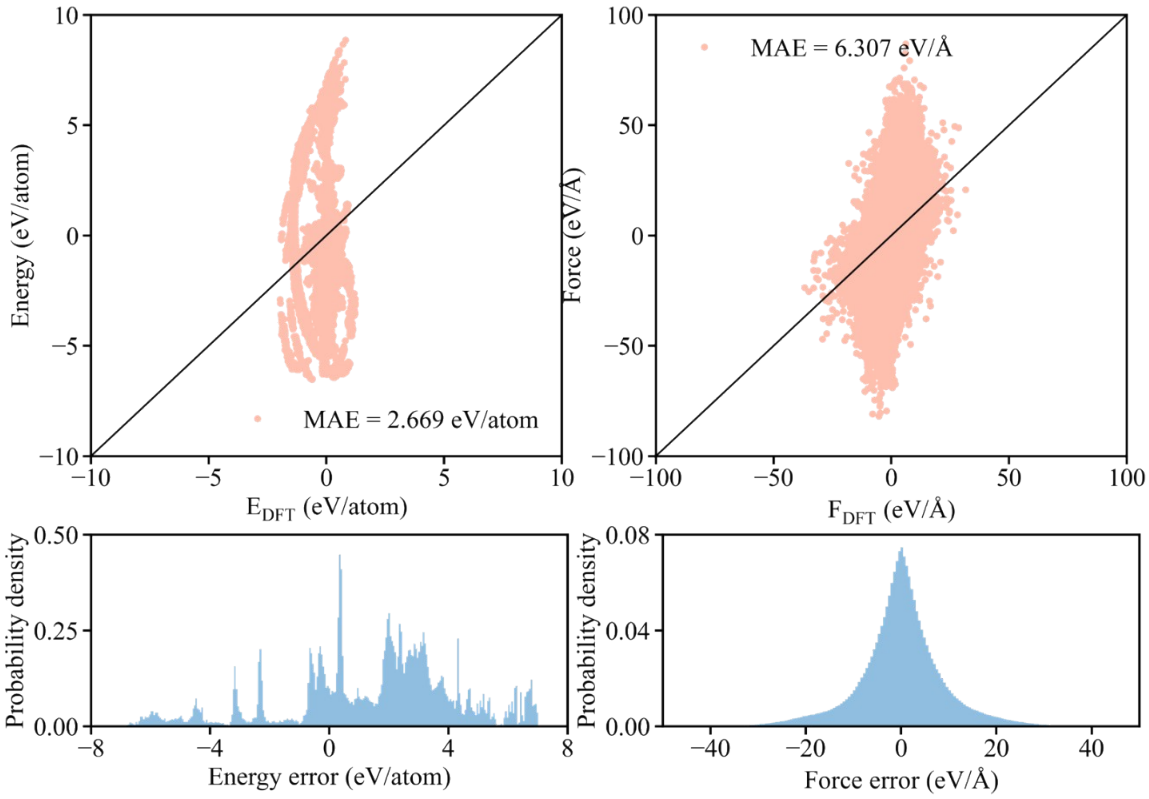

Figure S4. Mean absolute errors of energy and atomic force for ReaxFF model on the DFT database. Statistical information of prediction errors on (c) energies and (d) forces.

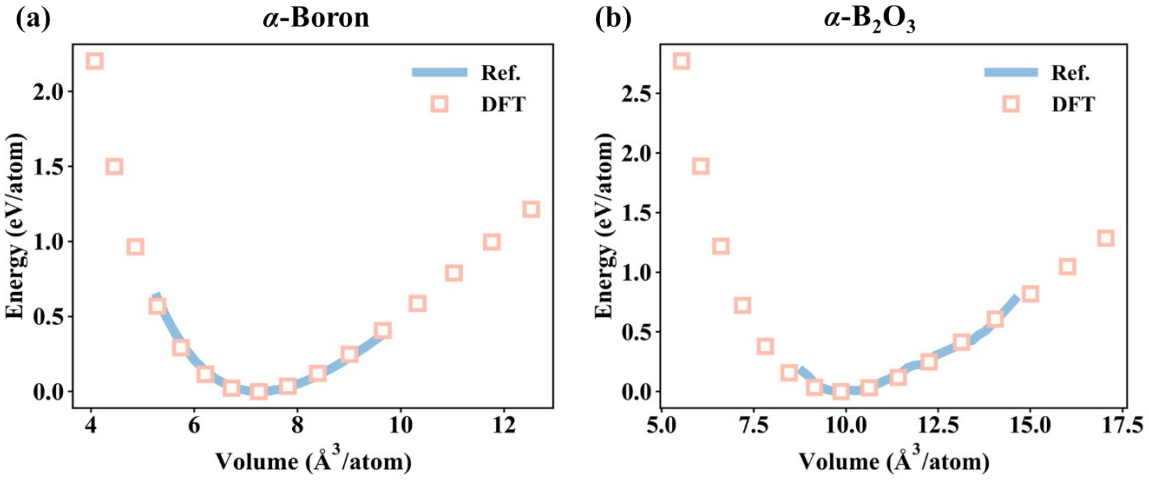

Figure S5. Equation of state curve for α-boron (a) and α-B_2O_3 crystals (b). The blue line and pink squares denote the literature values and DFT results, respectively. The scaling factor of the calculated structures ranges from 0.8-1.2.

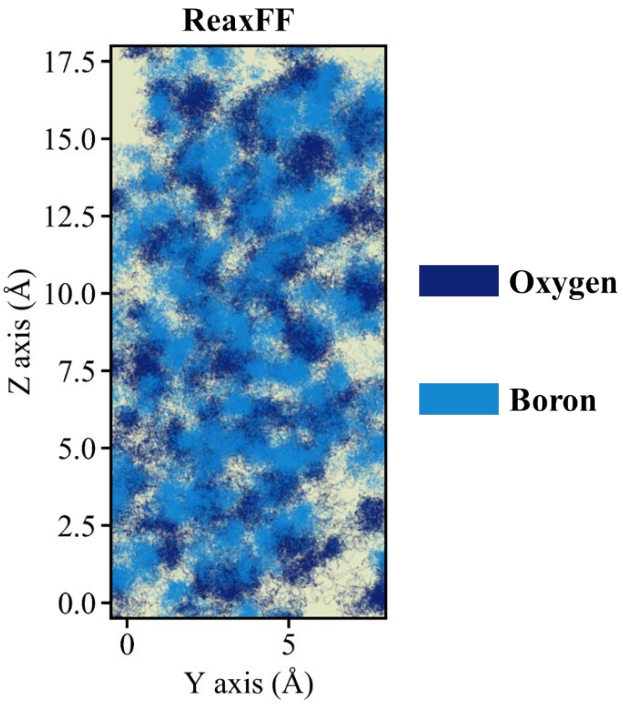

Figure S6. Projected coordinates for boron and oxygen atoms in α-B_2O_3 obtained from ReaxFF simulations with a timestep in 2 fs.

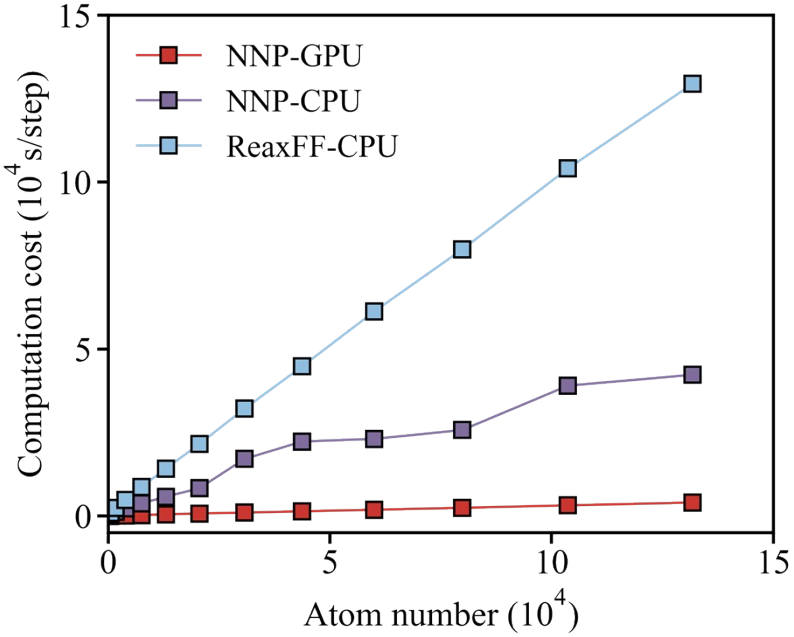

Figure S7. Computational cost of NNP-GPU (red square), NNP-CPU (purple square) and ReaxFF-CPU (blue square) methods on bulk α-B_2O_3 systems with 135 to 131820 atoms.