Supporting Information

Insight into the temperature-dependent lattice thermal properties of CeO_2 stabilized ZrO_2 by machine learning force field

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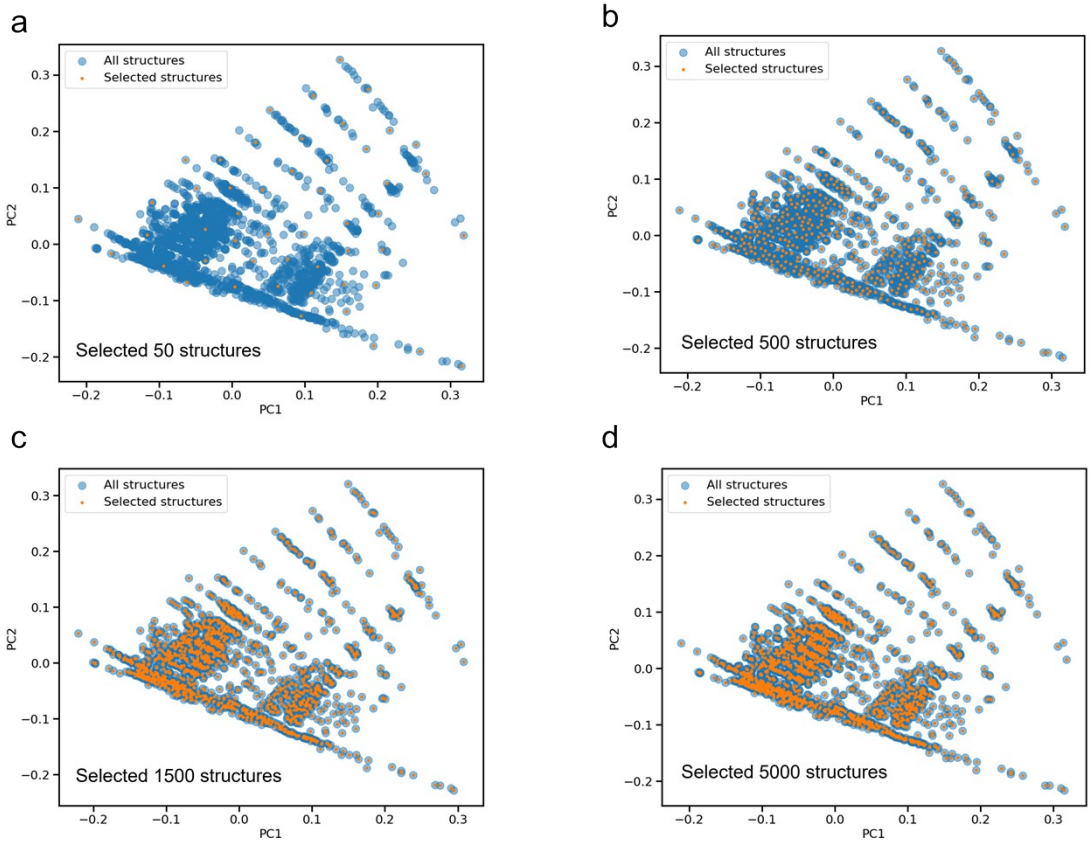

Fig.S1. A schematic diagram composed of 12303 structures in the dataset. Each orange dot represents the atomic configuration sampled by the FPS method. (a-d) represent sampling 50, 500, 1500, 5000, respectively.

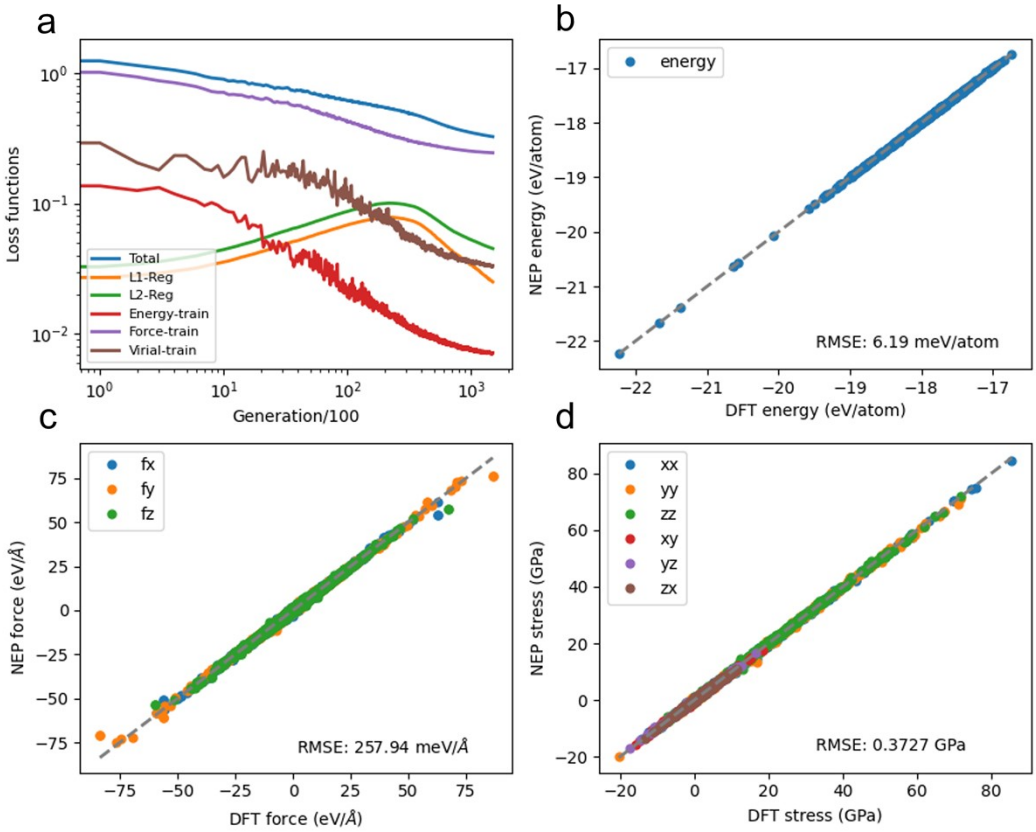

Fig.S2. (a) The loss function during the NEP training process; (b-d) Comparison between DFT and NEP prediction of energy, force, and stress in the testing dataset.

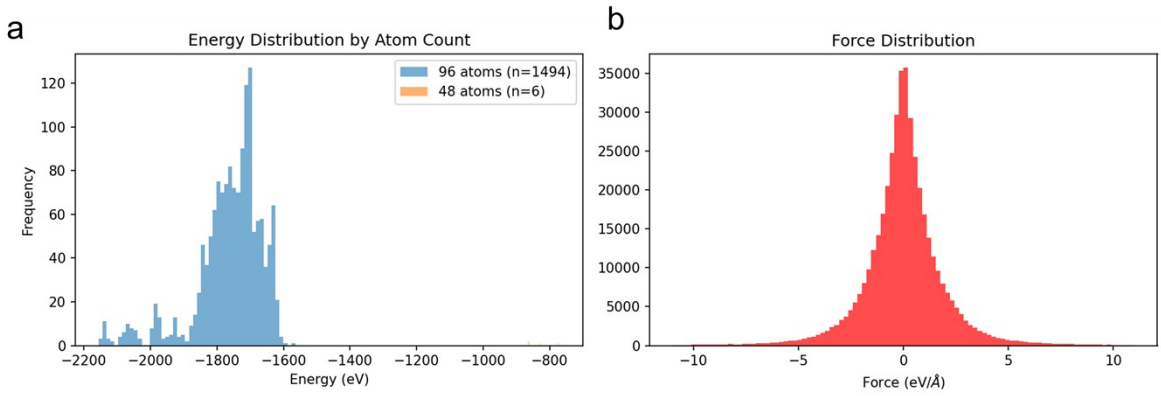

Fig. S3. Frequency distribution of energy and force in the dataset.

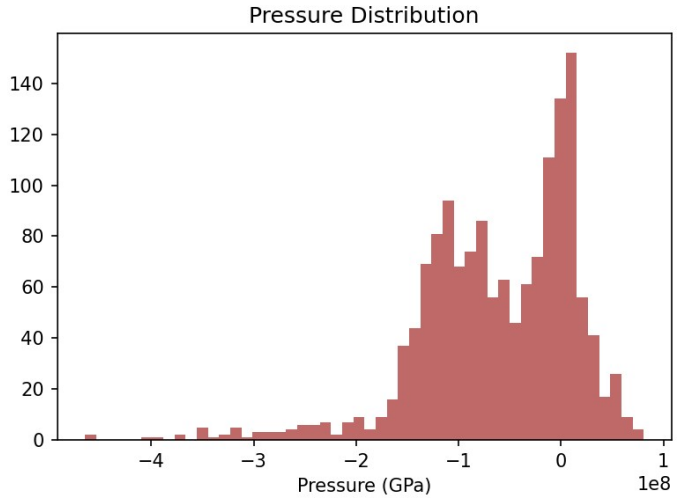

Fig. S4. Frequency distribution of pressure in the dataset.

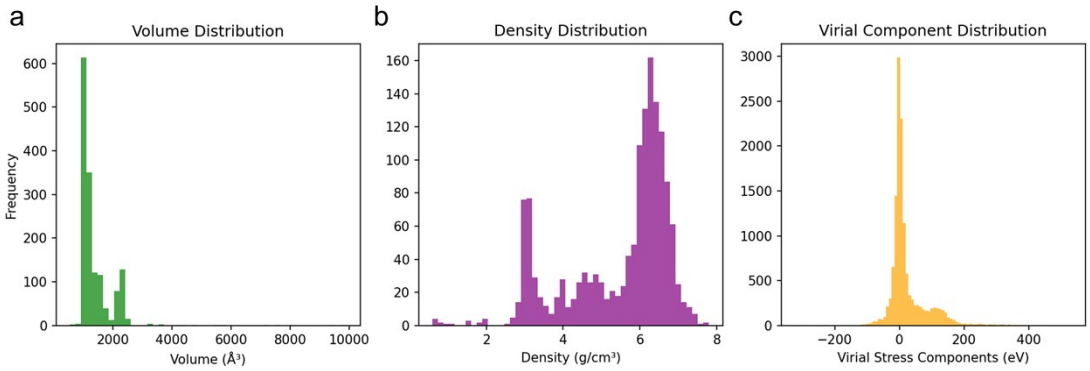

Fig. S5. Frequency distribution of dataset volume, density, and virial.

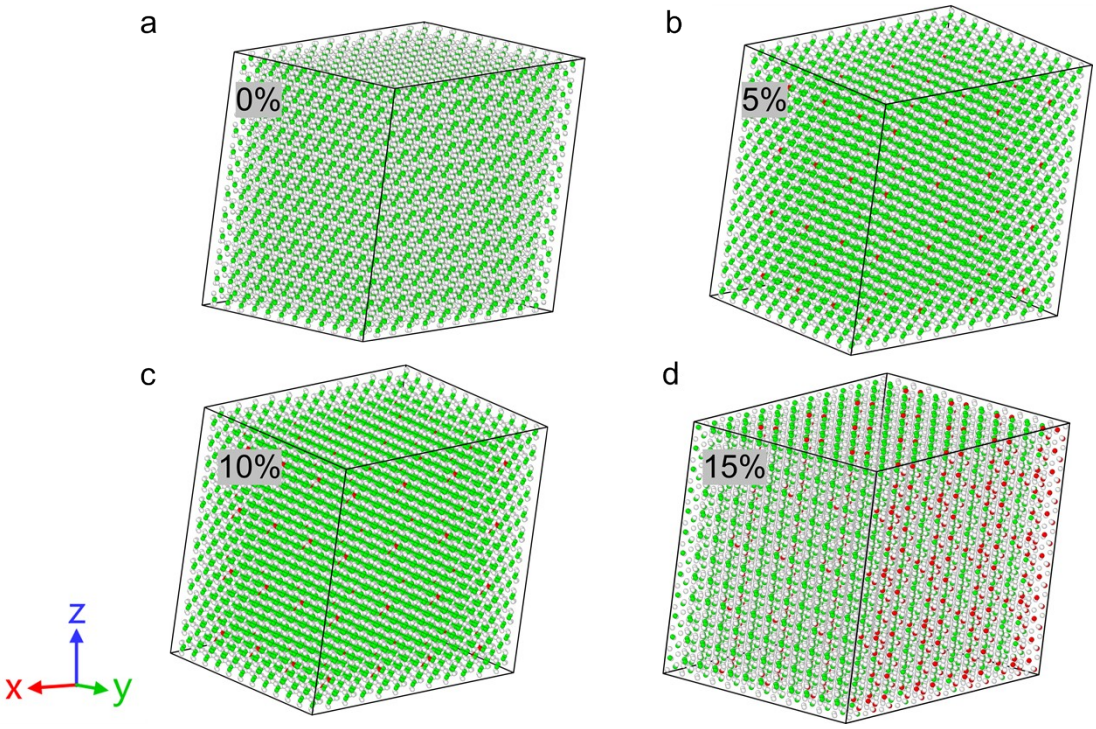

Fig. S6. Schematic diagram of monoclinic ZrO_2-CeO_2 structure with doping ratios of 0%, 5%, 10%, and 15%, respectively.

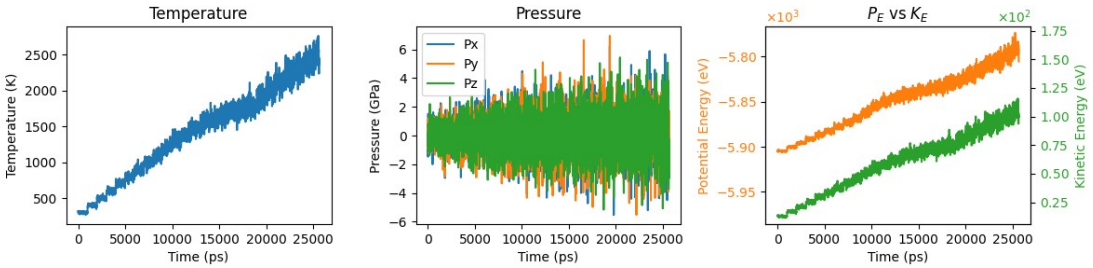

Fig. S7. The changes in temperature, pressure, and potential (kinetic) energy of the ZrO_2-CeO_2 structure with a doping ratio of 5%.

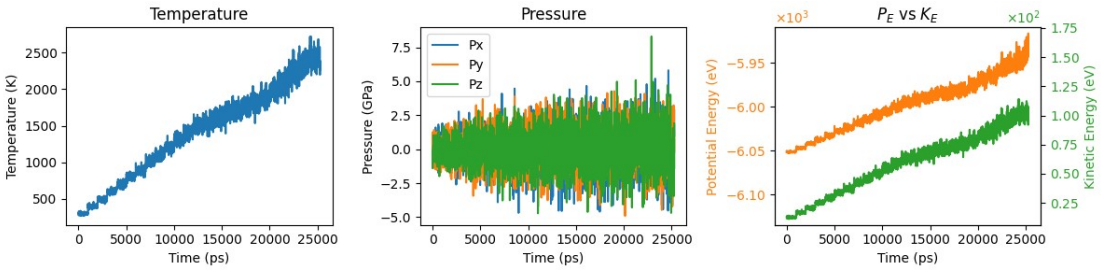

Fig. S8. The changes in temperature, pressure, and potential (kinetic) energy of the ZrO_2-CeO_2 structure with a doping ratio of 15%.

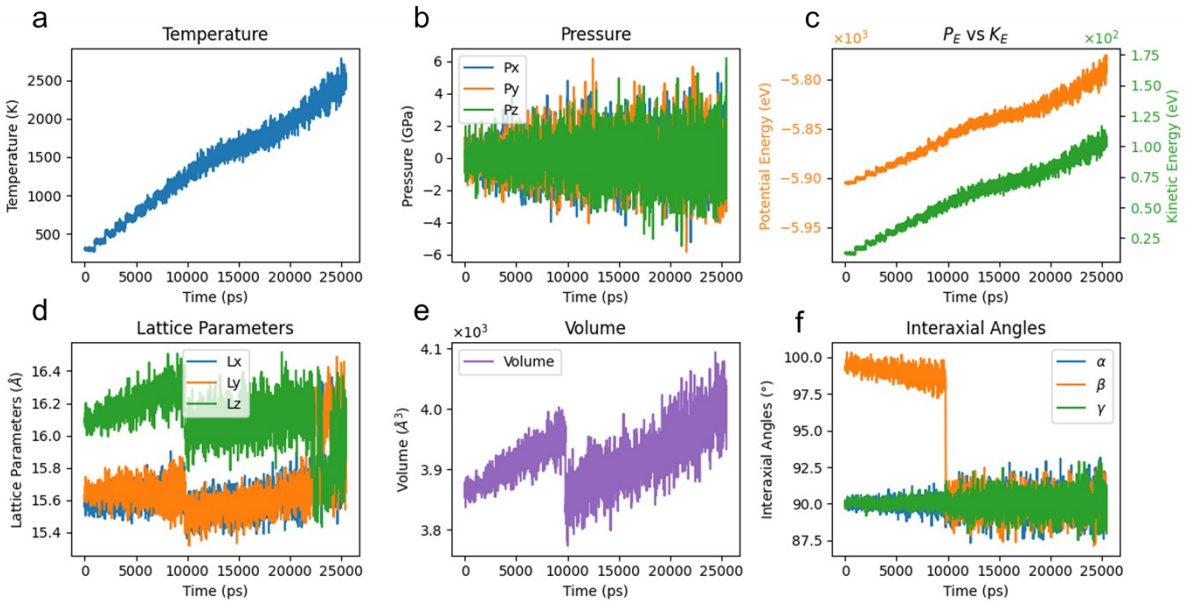

Fig. S9. The thermodynamic processes of the ZrO_2-CeO_2 structure with a doping ratio of 10%. (a-c) Changes in temperature, pressure, and potential (kinetic) energy over time. (d-f) The lattice parameters, volume, and angles over time.

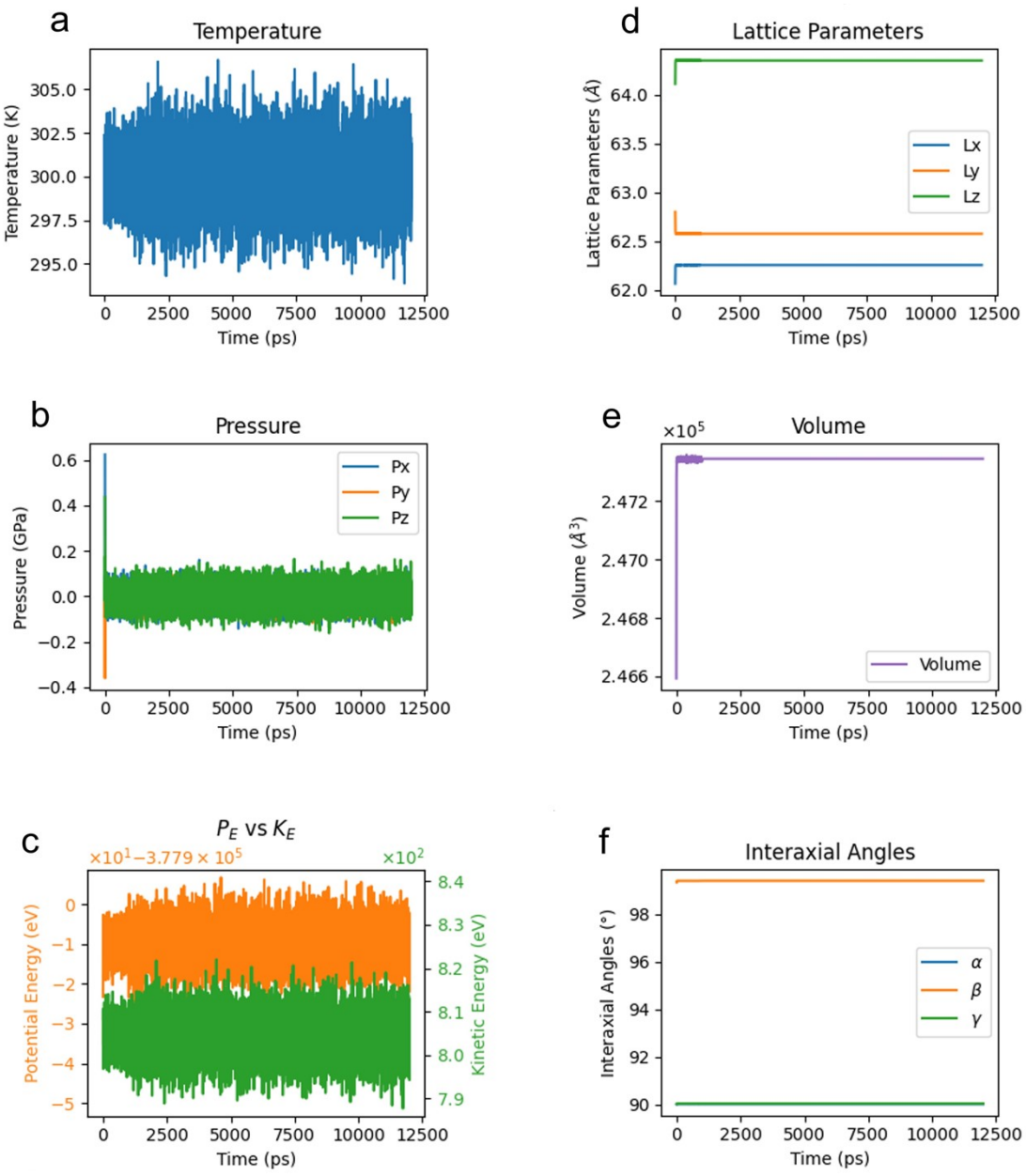

Fig. S10. Thermal stability during the relaxation process of a 5% doped structure.

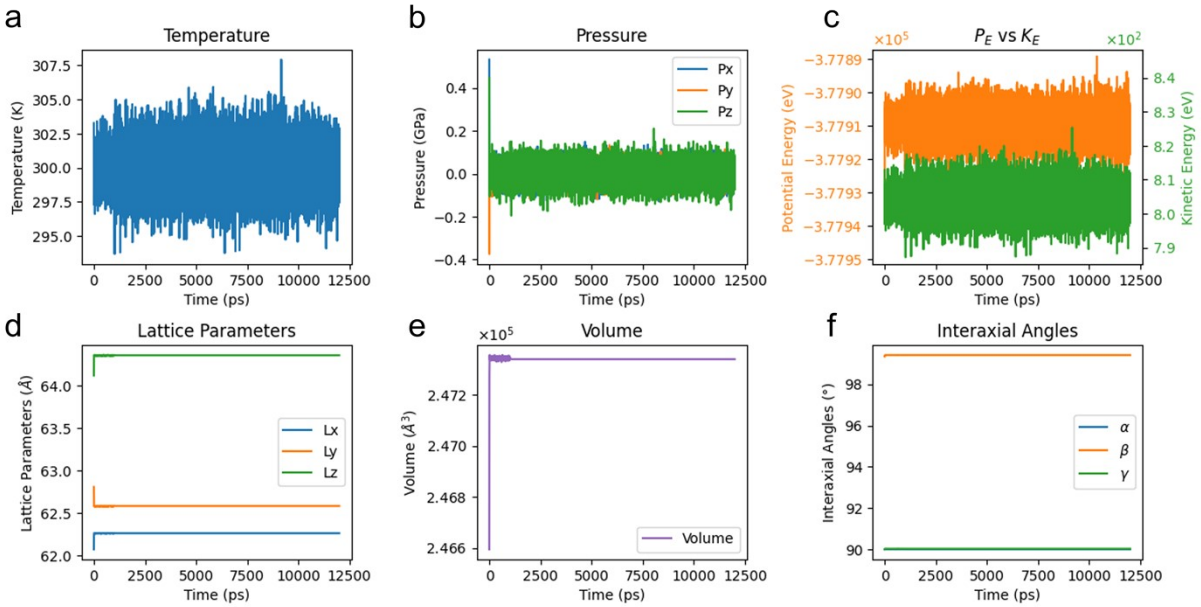

Fig. S11. Thermal stability during the relaxation process of a 10% doped structure.

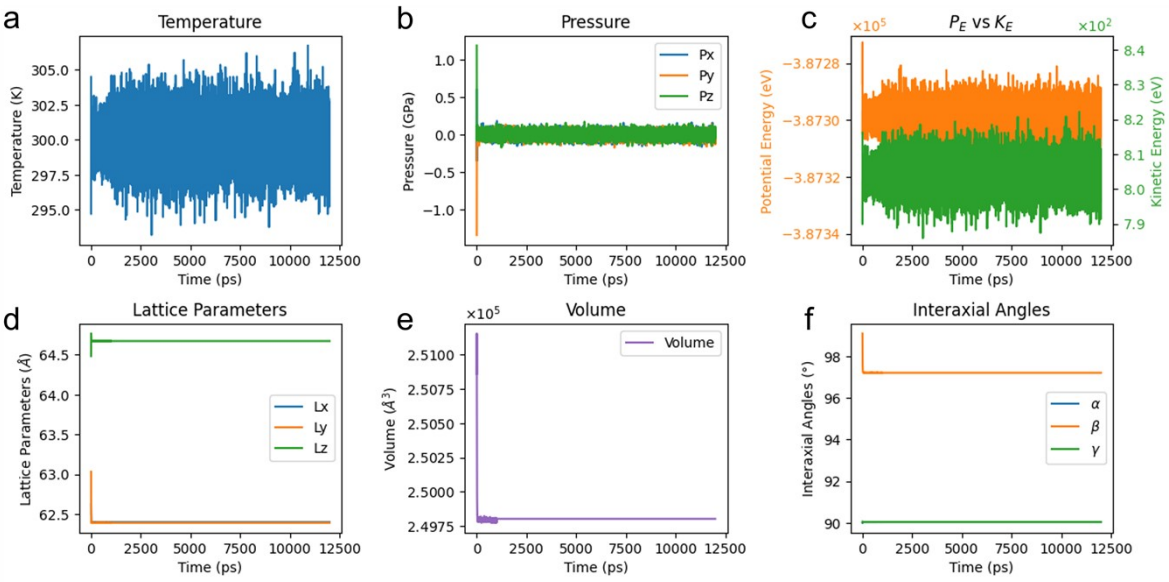

Fig. S12. Thermal stability during the relaxation process of a 15% doped structure.