Deep learning of accurate force field of $Hf_xSi_{1-x}O_2$

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1. Introduction

The HfO2 has become a potential material for the development of CMOS and nonvolatile memories due to its excellent dielectric and ferroelectric properties and silicon-compatible. Element doping can help regulate the stability of different phases of HfO2. Low-concentration silicon doping exhibits ferroelectric properties, while high-concentration Si doping promotes the formation of the t-phase structure with high dielectric constant. Using the DFT method, high-throughput screening of the effects of different element doping and doping concentrations on the stability of different HfO2 phases was found. The research revealed that Si doping significantly reduces the energy difference between the t-phase and the o-phase, and more effectively lowers the ferroelectric switching barrier, which is beneficial to its application in ferroelectric devices. By training the $Hf_xSi_{1-x}O_2$ machine learning potential using the DPGEN, a high-precision potential was obtained, enabling the investigation of its phase transition mechanism and polarization reversal dynamics from a molecular dynamics perspective.

2. Method

Based on our VASP calculations and the pure HfO_2 training dataset from Wu et al. [1], we trained a machine learning potential for $Hf_xSi_{1-x}O_2$ (x=0-25%) using DP-GEN [2]. This potential achieves high accuracy (RMSE_E: 3.703 meV/atom; RMSE_F: 0.115–0.125 eV/Å) and is applied to simulations of a 6144-atom supercell. This enables large-scale phase stability and polarization dynamics research under silicon-doped conditions, guiding the design of HfO_2-based ferroelectric devices.

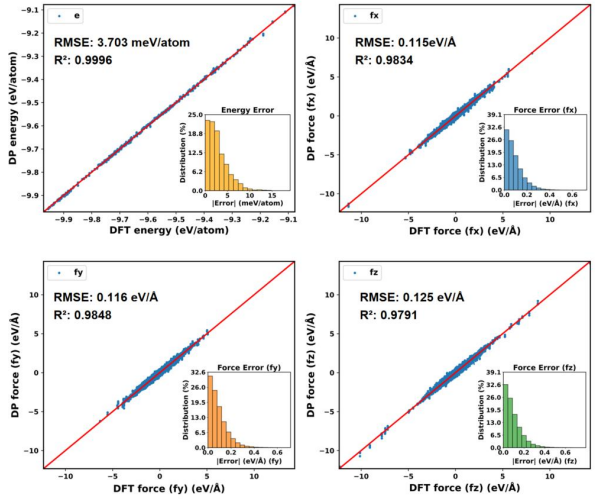

Fig. 1: Accuracy of DPGEN-Trained Potential: Energy and Force Predictions

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