Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Simulating Isotropic Raman Spectra of O-H Stretching Mode in Liquid H_2O based on a Machine Learning Potential: the Influence of Vibrational Couplings

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Supporting Information

Figure S1. Learning curves of (A) energy and (B) force for training set in terms of RMSE.

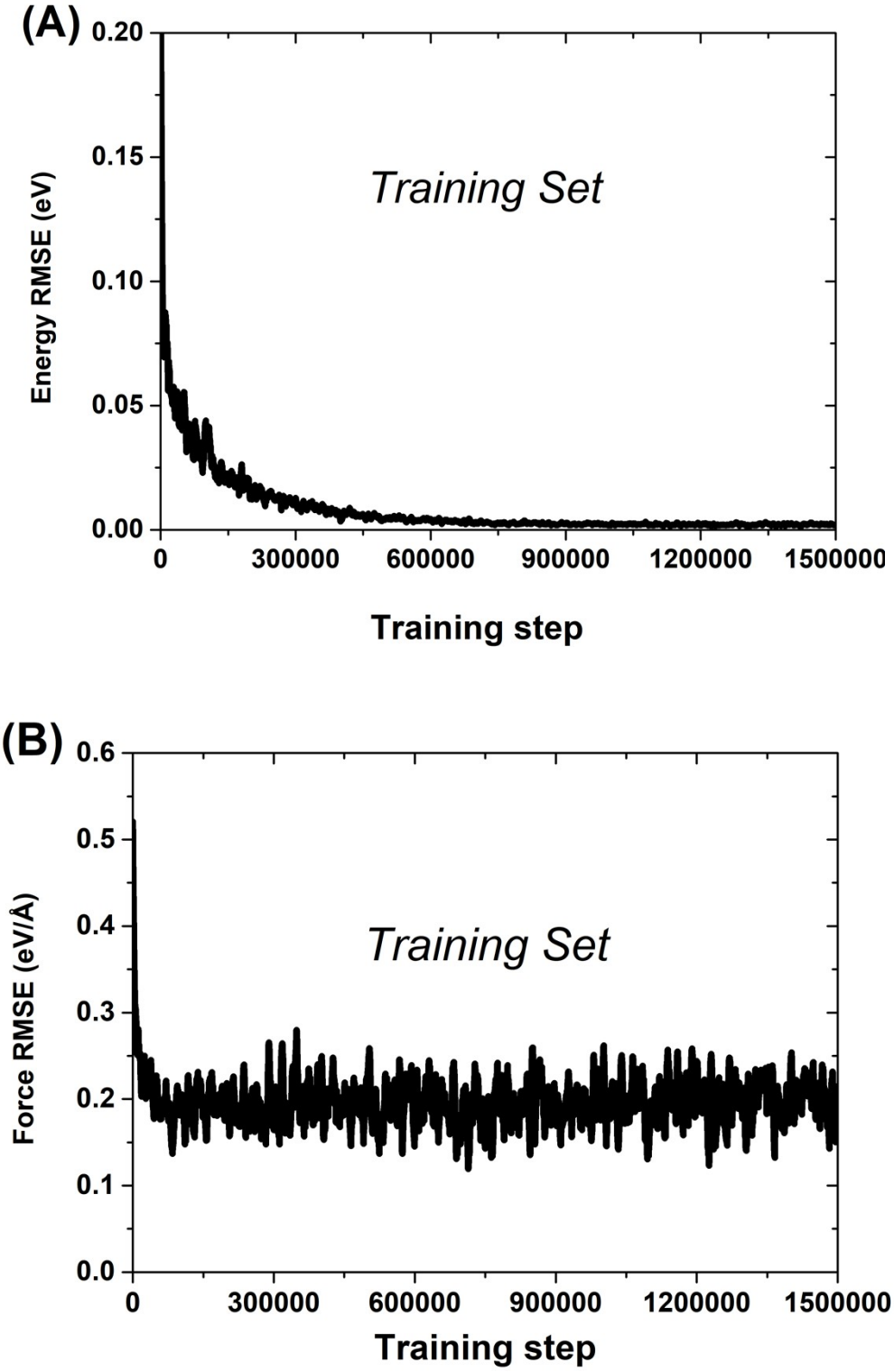

Figure S2. Learning curves of (A) energy and (B) force for validation set in terms of RMSE.

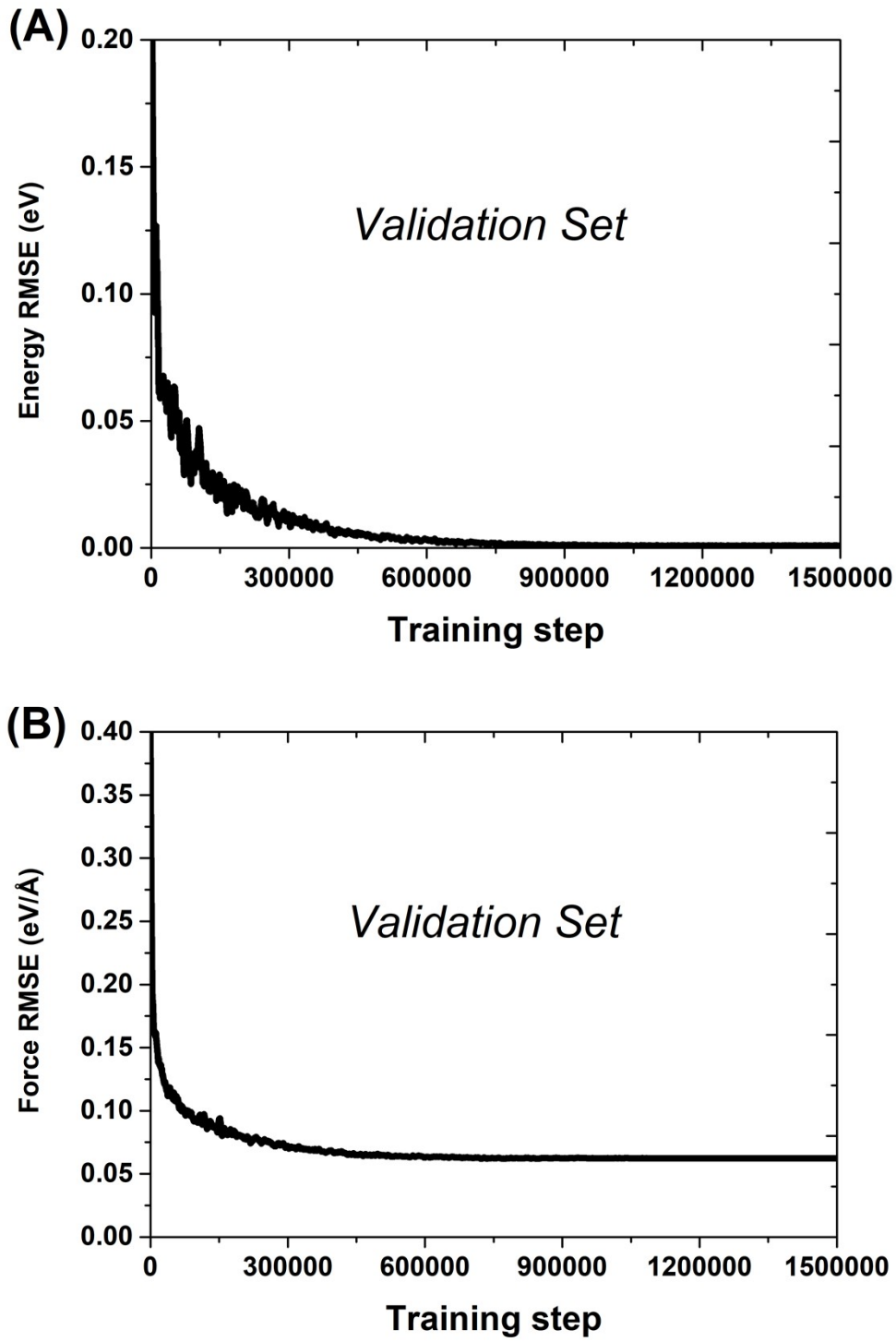

Figure S3. Radial distribution functions (RDFs) of (A) H-H, (B) O-H, (C) O-O, obtained from DFT-MD (SCAN) and DeePMD simulations (64 and 512 water molecules).