

Supplementary information

Investigation of phase transition, mechanical behavior and lattice thermal conductivity on halogen perovskite using machine learning interatomic potentials

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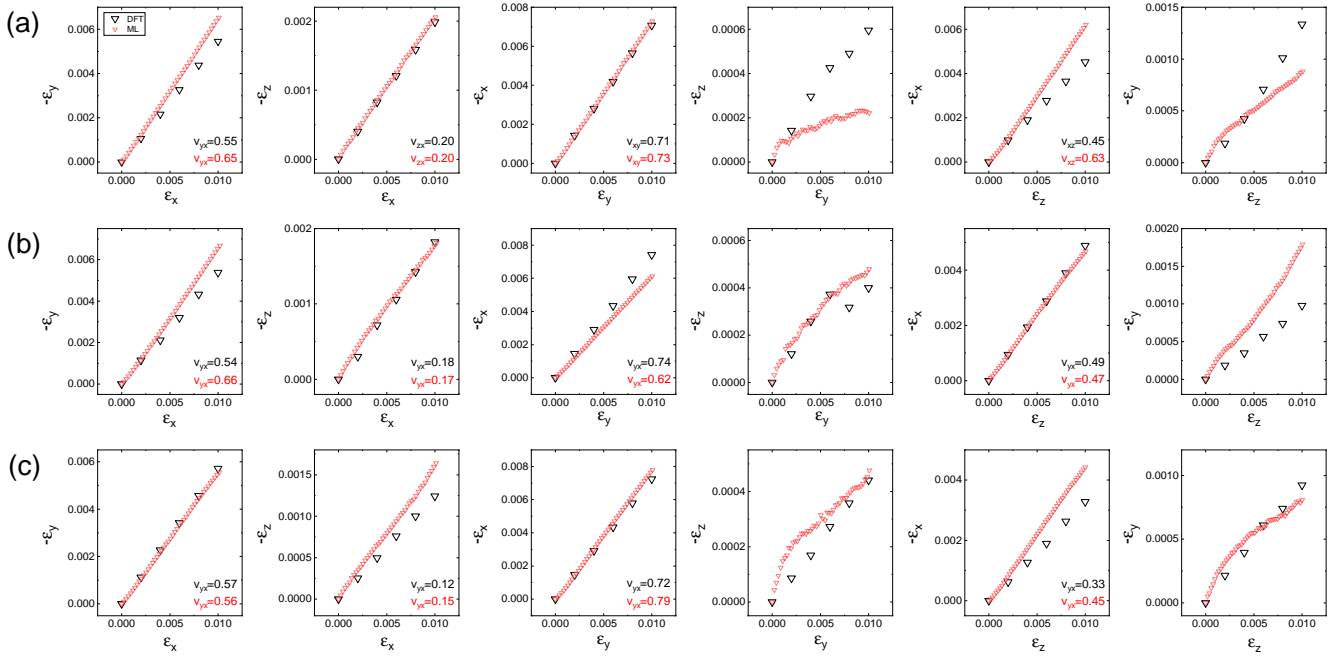


Figure S1. The correlations between the transverse strains (longitudinal coordinates) and applied uniaxial strains (horizontal coordinates) for CsPbX₃ (X=Cl, Br and I), (a) CsPbCl₃, (b) CsPbBr₃, (c) CsPbI₃. The black symbol gives the DFT result. The red symbol represents the NEP-based MD prediction with NpT ensemble at 0.1 K. Poisson's ratio is derived from the slope of the linear fitting, as shown in figure.

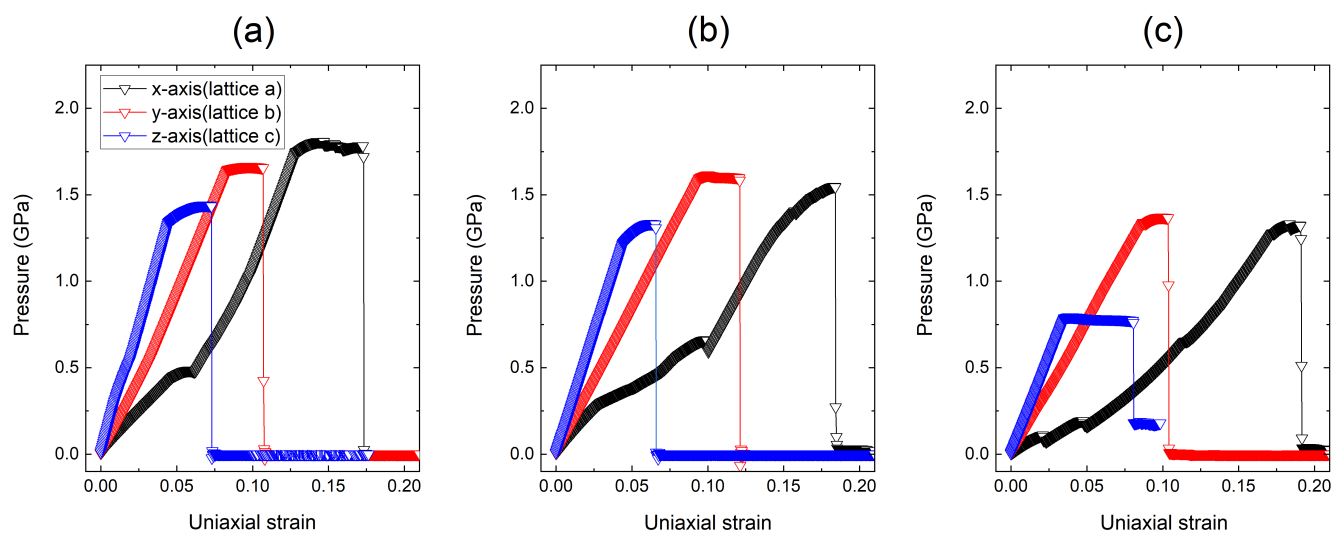


Figure S2. Pressure as a function of uniaxial strain for CsPbX_3 ($X=\text{Cl}$, Br and I), (a) CsPbCl_3 , (b) CsPbBr_3 , (c) CsPbI_3 . The NEP-based MD simulations with NpT ensemble are performed in a large supercell containing 16000 atoms. The system at 0.10 K is first relaxed for 1 ns to obtain an equilibrium state, and then uniaxial strain is applied to the system with the deformation rate of 10^{-6} Å/step.

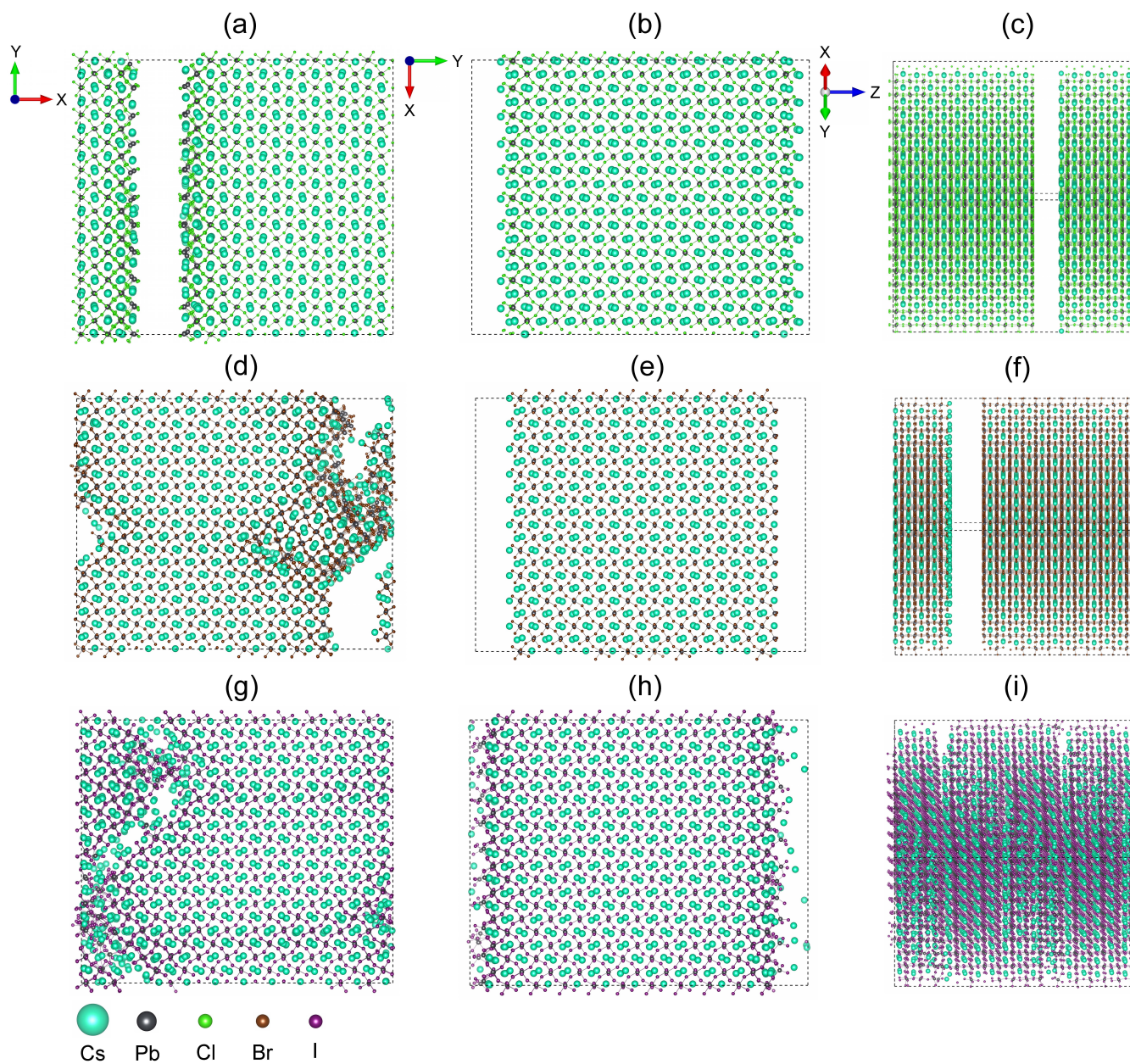


Figure S3. Rupture behavior of the CsPbX_3 predicted by NEP-based MD simulations with NpT ensemble. (a)-(c) for CsPbCl_3 , (d)-(f) for CsPbBr_3 , (g)-(i) for CsPbI_3 . (a)/(d)/(g), (b)/(e)/(h) and (c)/(f)/(i) represent the strain applied to the x , y and z -axis, respectively.

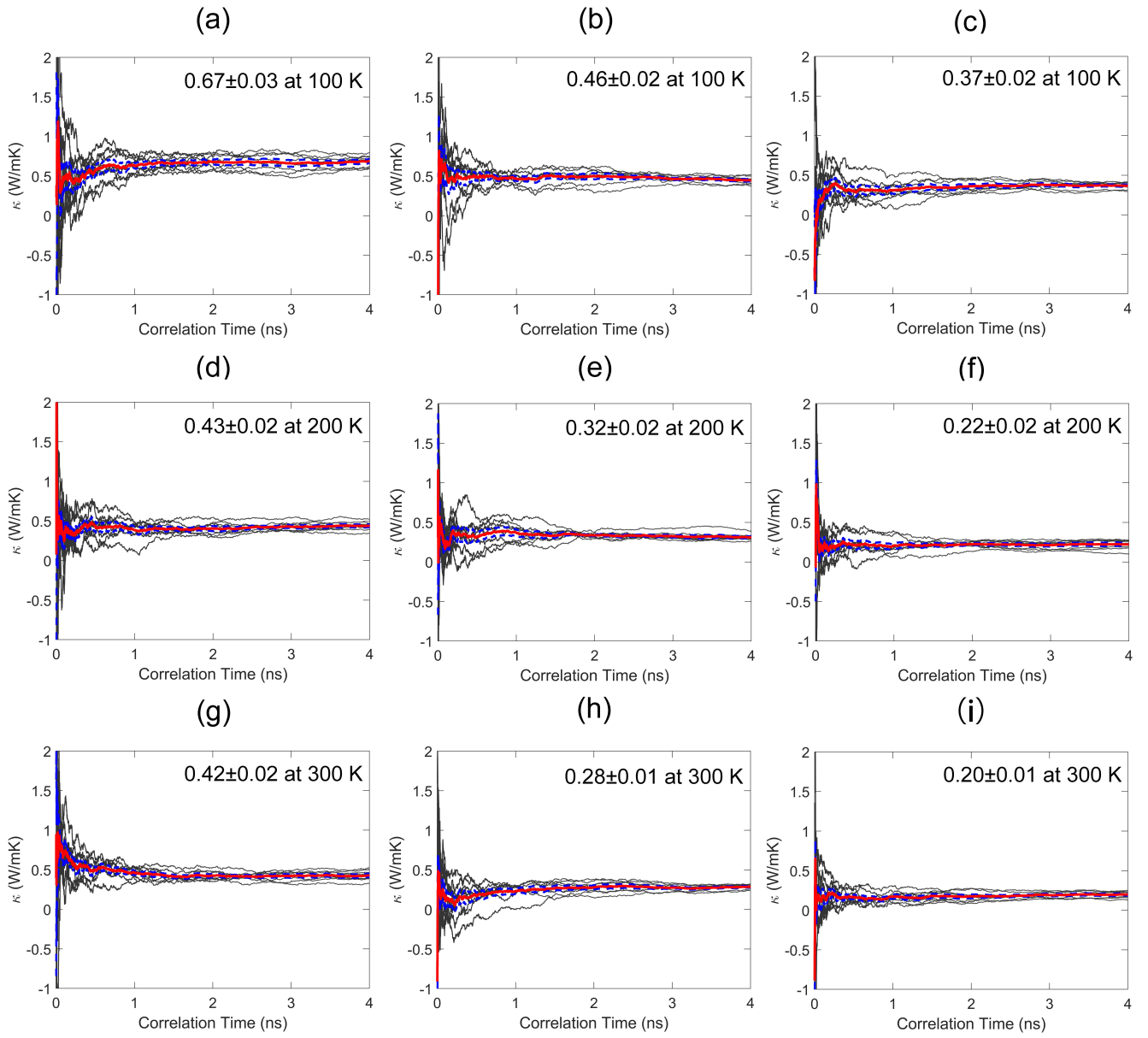


Figure S4. Lattice thermal conductivity of halogen perovskite along x -axis direction. The black, red solid and blue dashed lines represent 8 independent running, their average value and error bounds, respectively. (a)/(d)/(g), (b)/(e)/(h) and (c)/(f)/(i) represent the results of CsPbCl_3 , CsPbBr_3 , CsPbI_3 , respectively.

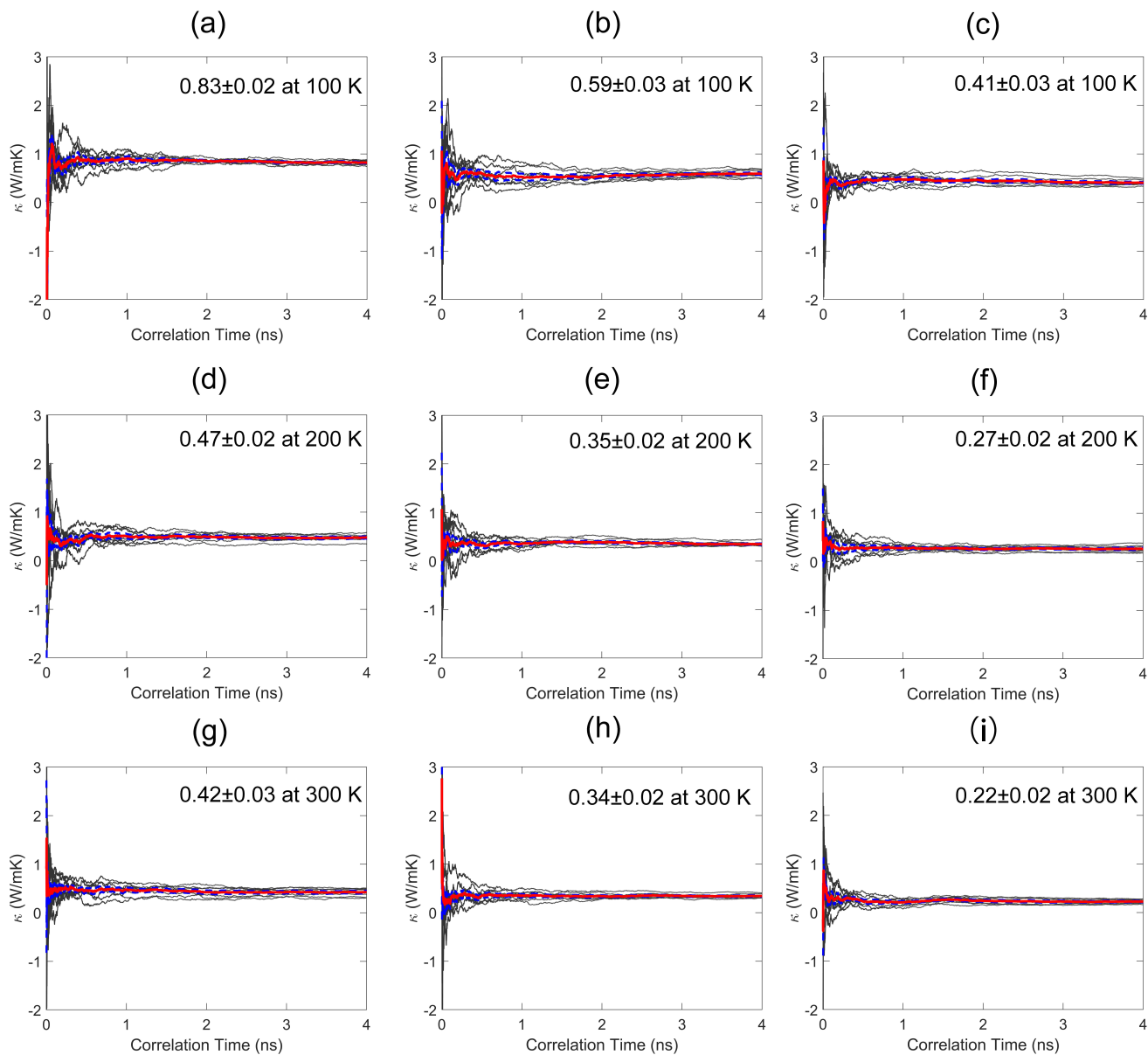


Figure S5. Lattice thermal conductivity of halogen perovskite along z -axis direction. The black, red solid and blue dashed lines represent 8 independent running, their average value and error bounds, respectively. (a)/(d)/(g), (b)/(e)/(h) and (c)/(f)/(i) represent the results of CsPbCl_3 , CsPbBr_3 , CsPbI_3 , respectively.

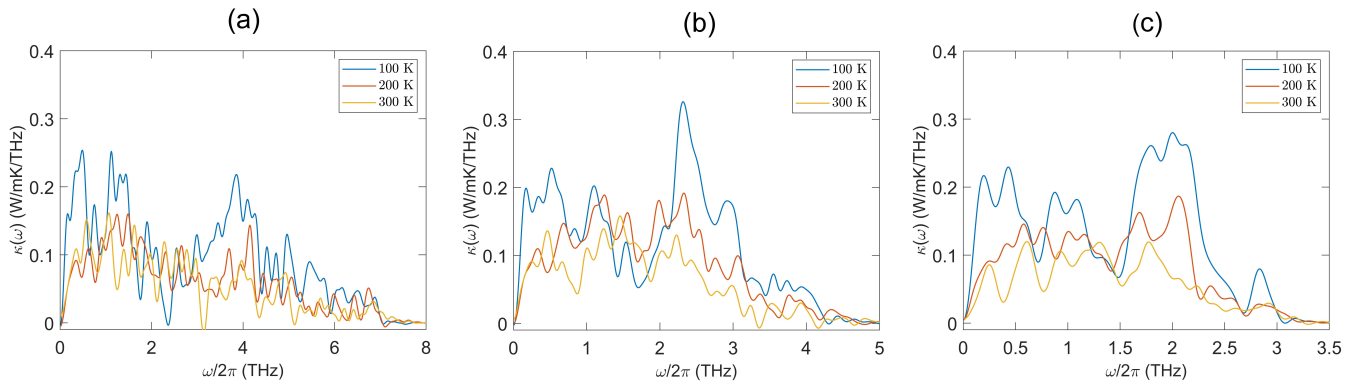


Figure S6. The spectral thermal conductivity of halogen perovskite. (a), (b) and (c) represent the results of CsPbCl_3 , CsPbBr_3 , CsPbI_3 , respectively.