Supplemental Materials for

Phonon thermal transport in Bi_2Te_3/Sb_2Te_3 monolayer superlattice: a neural network potential study

Pan Zhang,[a,b] Fang Lyv,[b] Dan Jin,[b] Zhenhua Zhang,[c] Shiwei Chen,[a] Yong Liu,[b] Ziyu Wang,[b] Zhihong Lu,[c] Shiheng Liang *[a] and Rui Xiong *[b]

a. School of Physics, Hubei University, Wuhan 430062, People's Republic of China

b. Key Laboratory of Artificial Micro- and Nano-structures of Ministry of Education, School of Physics and Technology, Wuhan University, Wuhan 430072, People's Republic of China

c. The State Key Laboratory of Refractories and Metallurgy, School of Materials Science and Engineering, Wuhan University of Science and Technology, Wuhan 430081, People's Republic of China

Corresponding author: Shihengliang@hubu.edu.cn

Corresponding author: xiongrui@whu.edu.cn

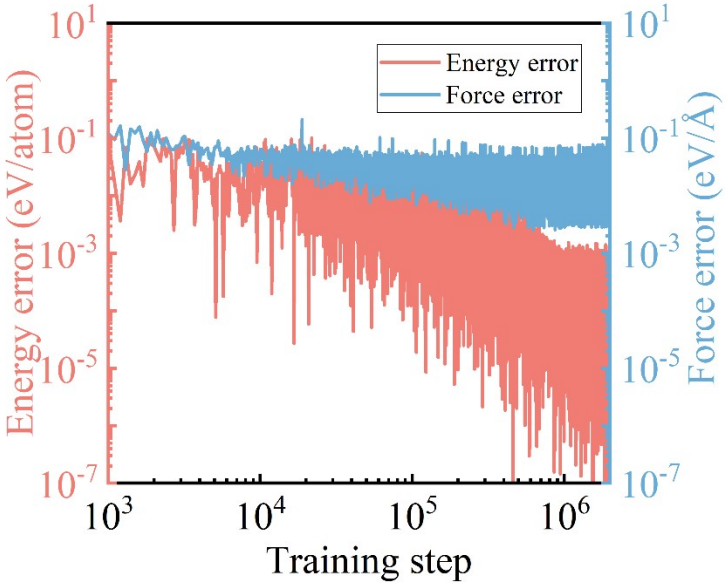

Fig. S1 The loss functions of energy and force during training process.

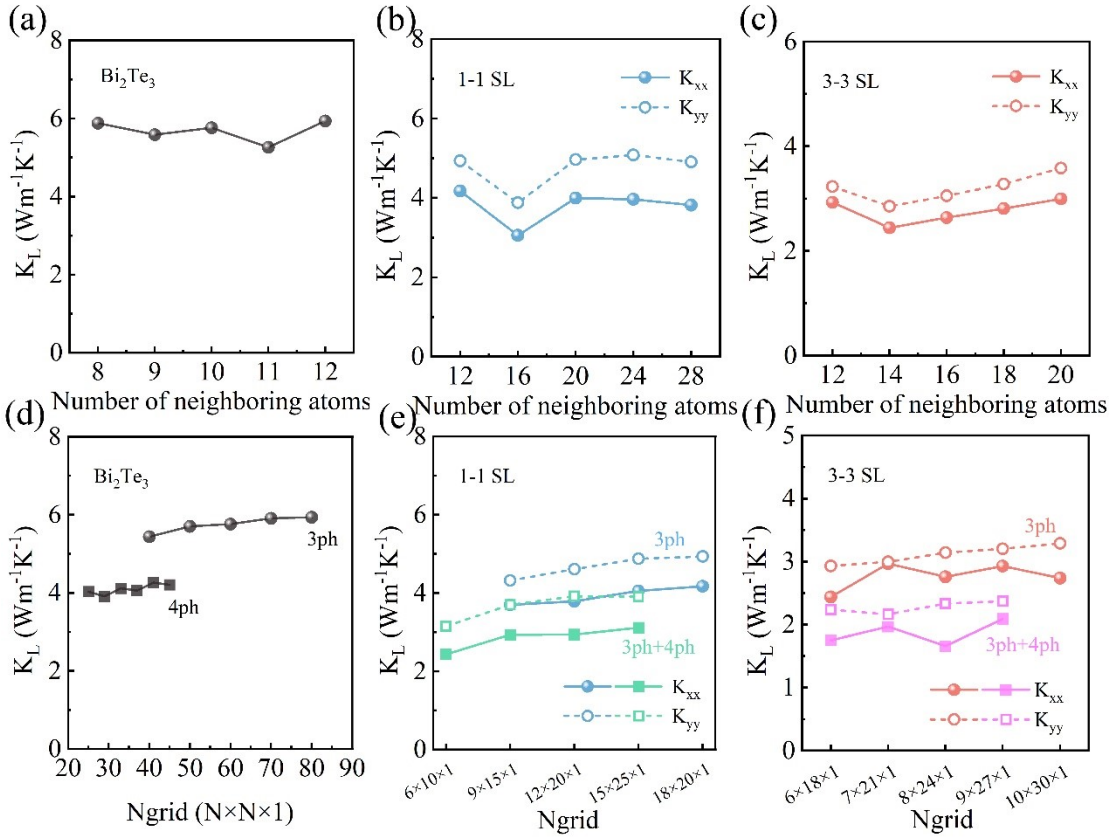

Fig. S2 Convergence tests of (a-c) number of neighboring atoms and (d-f) q-mesh in the Brillouin zone for solving phonon Boltzmann transport equation in the calculation of lattice thermal conductivity of Bi_2Te_3 monolayer, 1-1 and 3-3 Bi_2Te_3/Sb_2Te_3 monolayer superlattices. The 12th neighboring atoms are chosen for the three-order

interatomic force constants calculations. 80×80×1 and 45×45×1 q-meshes are used to calculate thermal conductivity of Bi_2Te_3 monolayer, while 18×30×1 and 15×25×1 q-meshes are used for 1-1 Bi_2Te_3/Sb_2Te_3 monolayer superlattice, and 9×27×1 and 7×21×1 q-meshes are used for 3-3 Bi_2Te_3/Sb_2Te_3 monolayer superlattice, when only three-phonon scattering processes and both three-phonon and four-phonon scattering processes are being considered, respectively, to obtain convergent results.

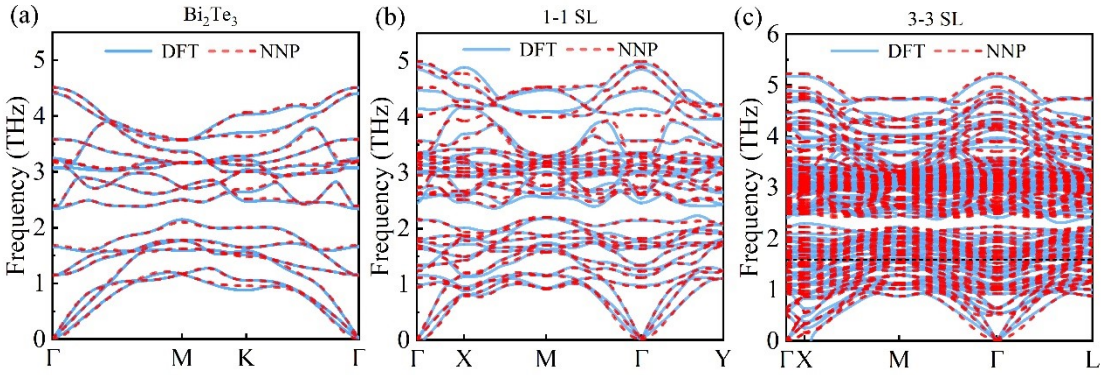

Fig. S3 (a) The phonon dispersions of (a) Bi_2Te_3 monolayer, (b) 1-1 and (c) 3-3 Bi_2Te_3/Sb_2Te_3 monolayer superlattices calculated using DFT and NNP, respectively.

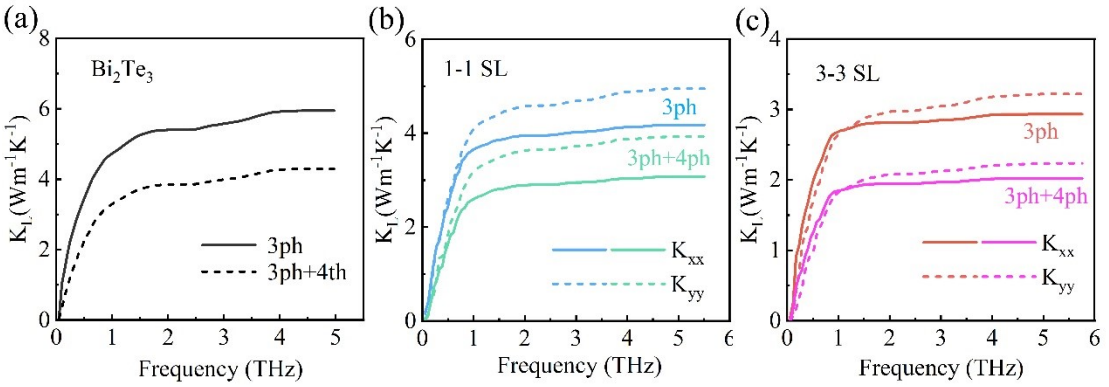

Fig. S4 (a) The cumulative lattice thermal conductivities at 300 K of (a) Bi_2Te_3 monolayer, (b) 1-1 and (c) 3-3 Bi_2Te_3/Sb_2Te_3 monolayer superlattices, respectively.