Supplementary Information: Neural Network Interatomic Potential for Laser-Excited Materials

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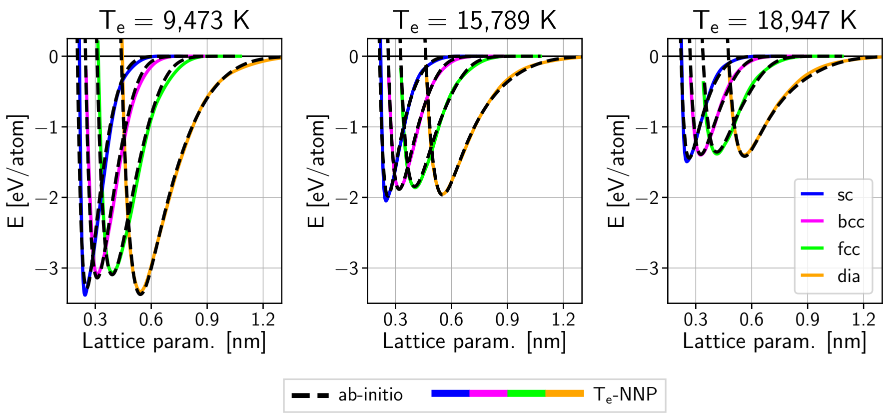

Fig. 1 Cohesive energy curves at other electronic temperatures. The Helmholtz free cohesive energy per atom at three different electronic temperature T_{e} as a function of the lattice parameter for different crystal structures. The ab-initio results obtained with DFT (CHIVES) are shown in black (dashed lines) and the results obtained with the T_{e}-NNP are colored.

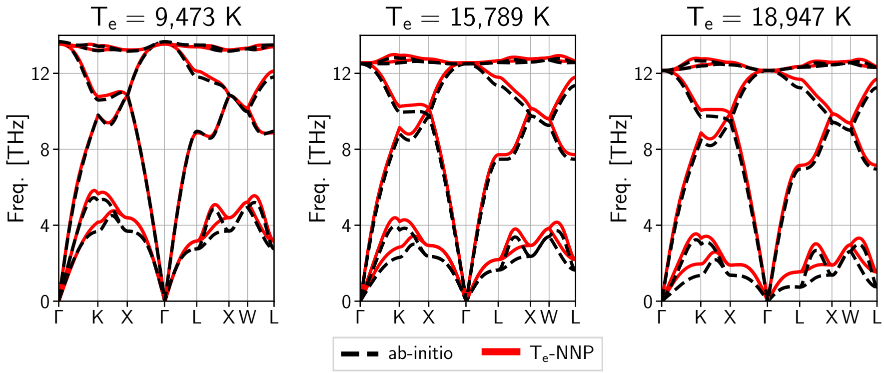

Fig. 2 Phonon band structures at other electronic temperatures. The phonon band structure of bulk diamond Si at three different electronic temperatures T_e. The ab-initio results obtained with DFT (CHIVES) are shown in black (dashed lines) and the results obtained with the T_e-NNP are colored red.

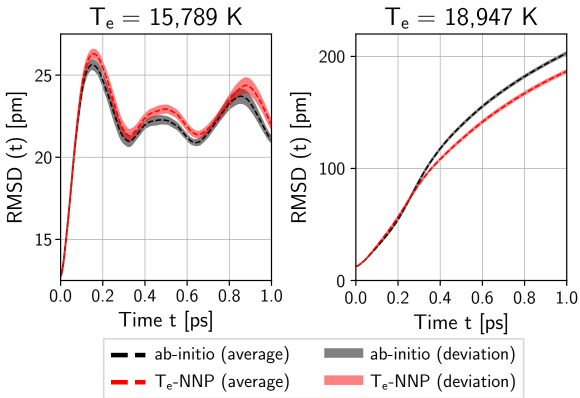

Fig. 3 Atomic root-mean-square displacements during MD simulations of bulk Si at other electronic temperatures. The root-mean-square displacements (RMSDs) of the Si atoms as a function of time after the laser excitation at two different electronic temperatures T_e. The ab-initio results obtained with DFT (CHIVES) are shown in black and the results obtained with the T_e-NNP are colored red. The width of the curves corresponds to twice the standard error of the mean over N simulation runs ($N = 10$ for $T_e = 15,789$ K and $N = 40$ for $18,947$ K).

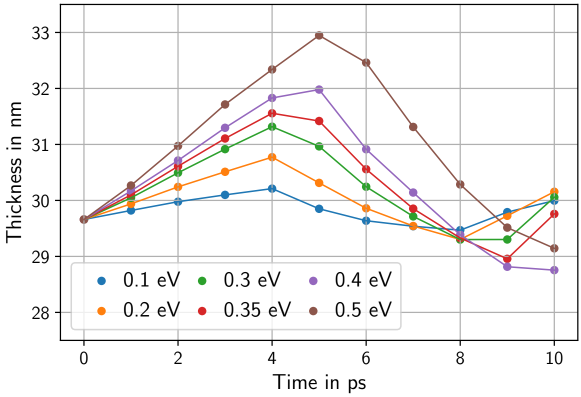

Fig. 4 Time evolution of thin film thickness. The time evolution of the thickness of the Si thin film during the large-scale MD simulations with the T_e-NNP for different pulse energies. Each thickness value corresponds to the average over two simulation runs (hill- and sink-like surface defect).

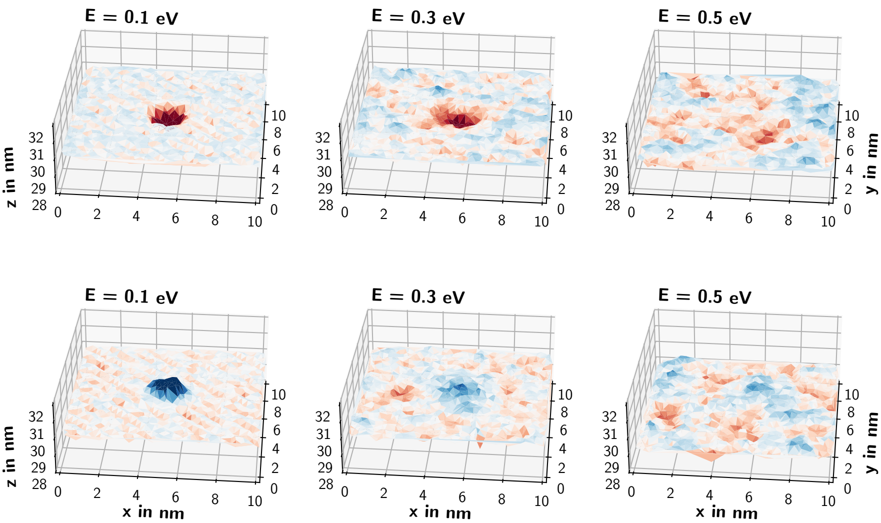

Fig. 5 Laser-induced surface modifications at other pulse energies. The top layer of two different Si thin films is shown at t = 10 ps after a laser excitation with different pulse energies. The upper row shows the top layer of a thin film with a sink-like surface defect, whereas the lower row shows a thin film with a hill-like surface defect. Both surface defects vanish within 10 ps for pulse energies above $E = 0.3$ eV. The MD simulations were performed using the T_e-NNP on a supercell containing more than 160,000 atoms.