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

Disperate effect of strain on thermal conductivity of 2-D materials

Supplementary Information

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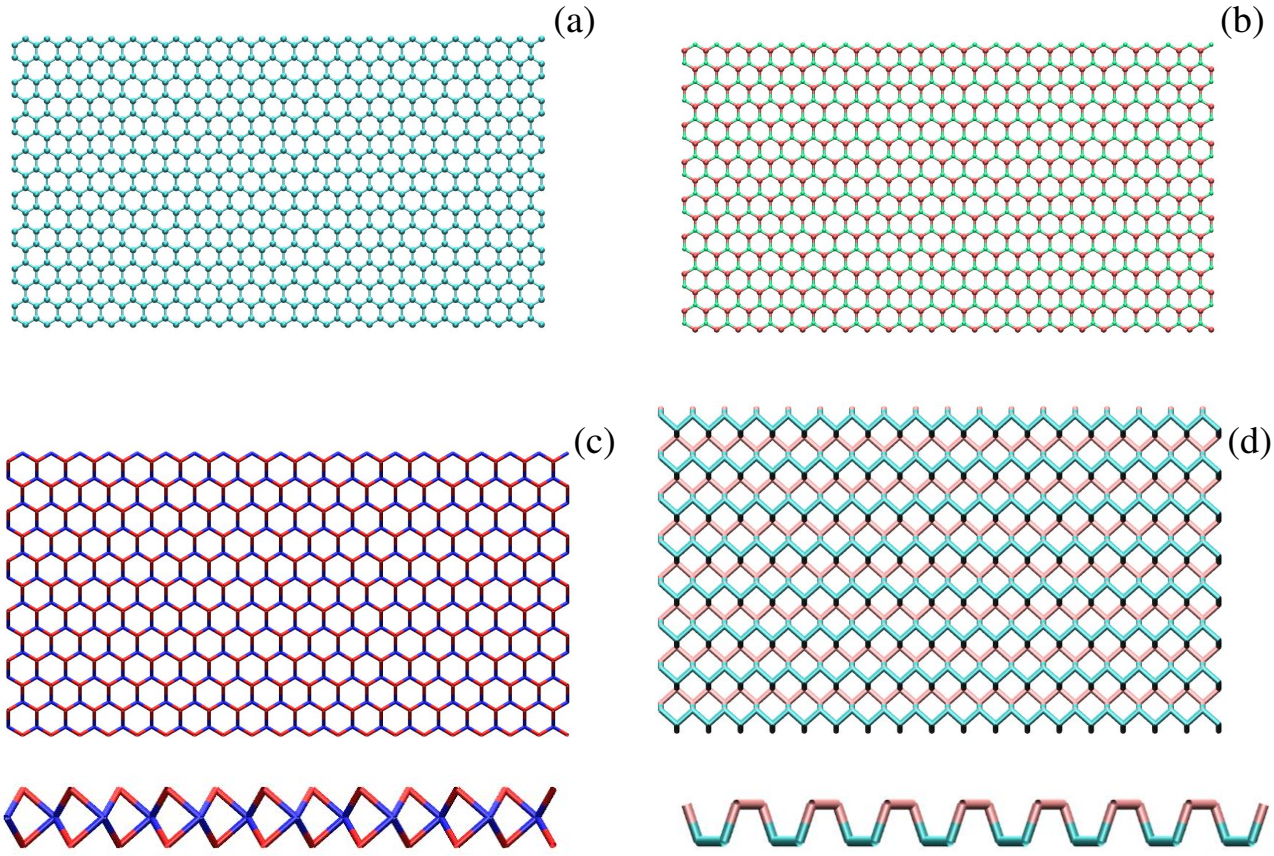

Figure 1: Atomic structures of zigzag (a) graphene (c) h-BN (c) MoS_2 (d) BP. Red and green color represent boron and nitrogen respectively in h-BN. Red and blue represent Sulphur and Molybdenum respectively in MoS_2. The bottom of the figures 1 (c),(d) represent the front view of MoS_2 and BP respectively.

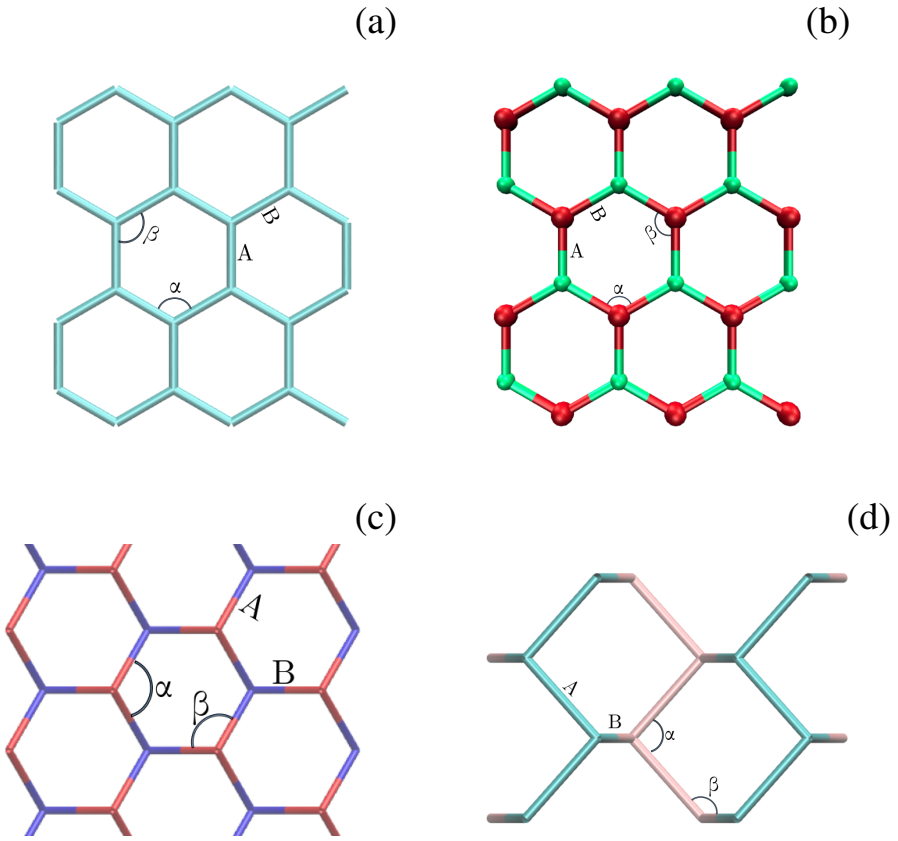

Figure 3: Different types of bond types and bond angles in (a) graphene (b)h-BN (c) MoS_2 (d) BP

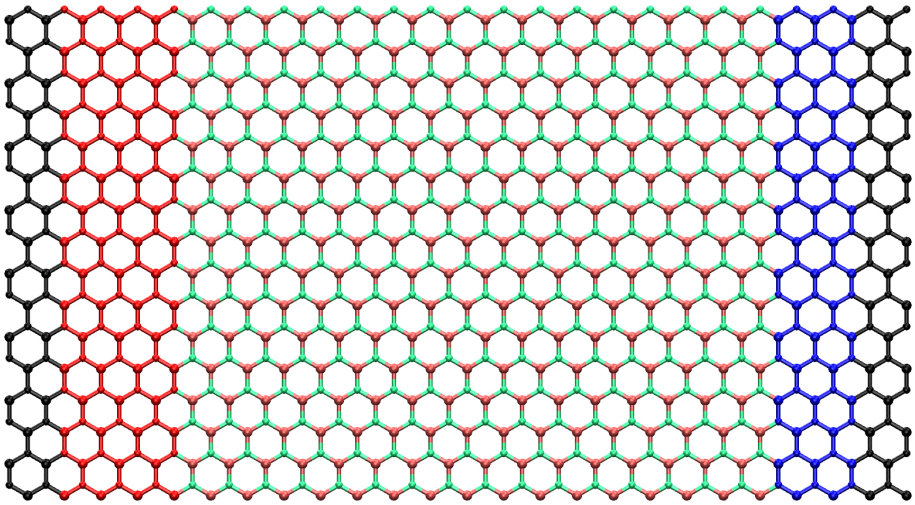

Figure 2: Schematic representation of NEMD in h-BN

Figure 2 represents the NEMD setup used in our simulations. Black region represents the fixed region. The red and blue represent the source and sink which are maintained at constant temperature of 320 and 280 K respectively.

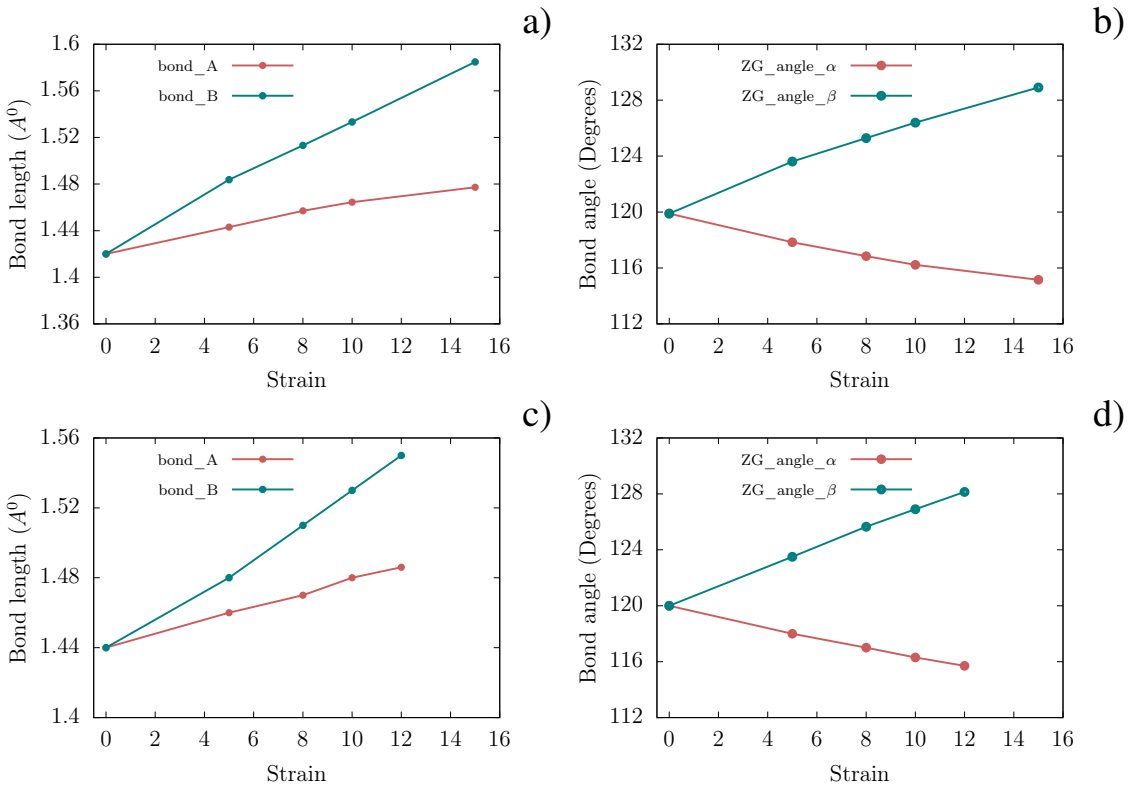

Figure 4: Variation of bond length and bond angles in (a), (b) graphene and (c), (d)h-BN

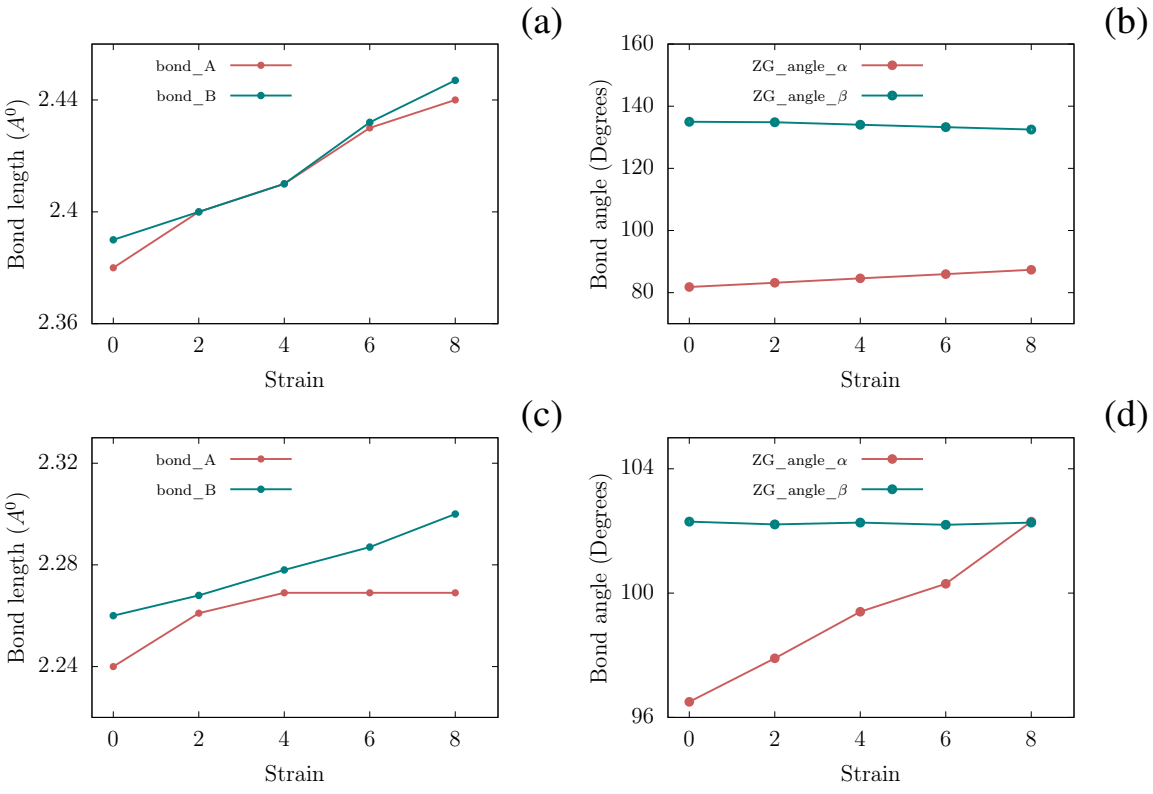

Figure 5: Variation of bond length and bond angles in (a),(b) MoS_2 and (c),(d) BP

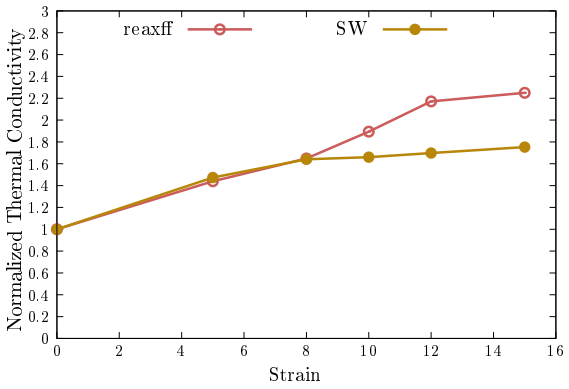

Figure 6: Variation of the thermal conductivity of silicene with strain using Reaxff and SW potential.

Spectral Energy Density of Phonons:

SED is formulated as,

$$\Phi(k,w) = \frac{m_b}{4\pi\tau_0 N_T} \sum_{\alpha} \sum_{b}^{n_b} |\int_0^{\tau_0} \sum_{l}^{N_T} \dot{u}_{\alpha}^{b,l}(t) exp[ik.r_0^l - i\omega t]dt|^2 \tag{1}$$

where, k represents the wave vector, ω is the angular frequency, m_b is the mass of the atom, N_T is the number of unit cells, τ_0 is the integration time, α represents direction, b is the basis atom, n_b is the number of basis atoms, and l is the index of the cell. $\dot{u}_{\alpha}^{b,l}$ is the velocity component of the basis atom of a cell along the α direction, r_0^l is the equilibrium position of the cell. The SED curves are fitted to Lorentzian curves to extract the relaxation time of phonons.

$$\Phi(k,\omega) = \frac{I}{1 + [(\omega - \omega_c)/\gamma]^2} \tag{2}$$

where, I is the magnitude of the peak and ω_c is the peak center frequency of the SED curves, and γ is the half-width of the peak at half maximum. The relaxation time of phonons is given by $\tau = 1/(2\gamma)$.

To calculate the SED curves, the system of size 10×10 nm^2 is considered for all the 2-D materials chosen. All the system are equilibrated in NPT ensemble for 2 ns. Then the systems were integrated in NVE ensemble for another 6 ns, where the last 4 ns data is used to compute the SED curves. The atomic postions and the velocities of the atoms are dumped at every 5 fs. The results presented are averaged over the 4 independent simulations. ΓX represents the zigzag direction in all the four 2-D materials.

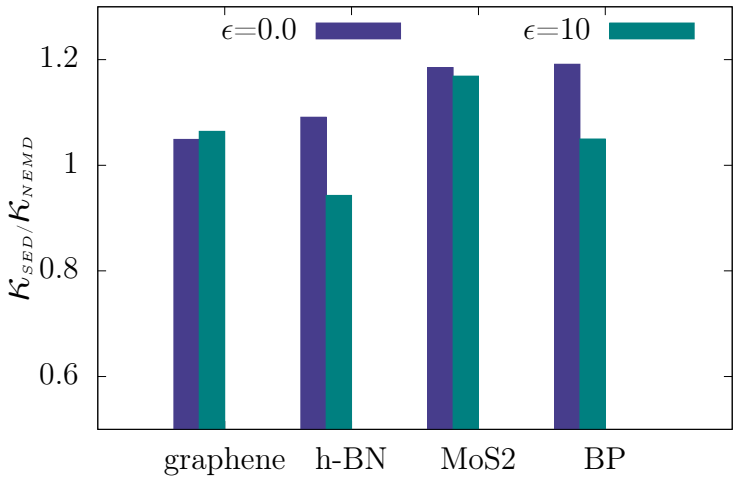

Figure 7: Comparison of κ values obtained from SED and NEMD simulations

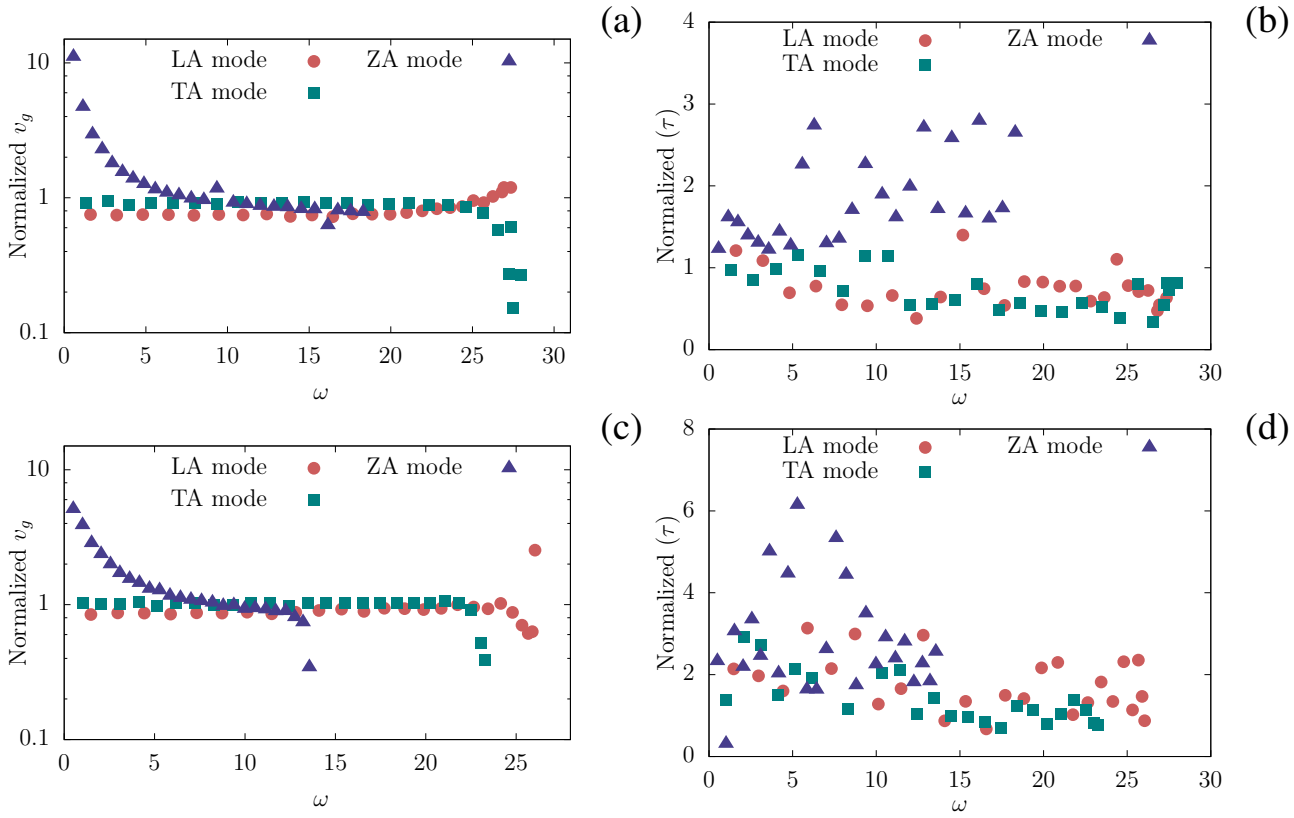

Figure 8: Normalized phonon group velocities of (a) graphene (c) h-BN. Normalized phonon relaxation time for (b) graphene (d) h-BN

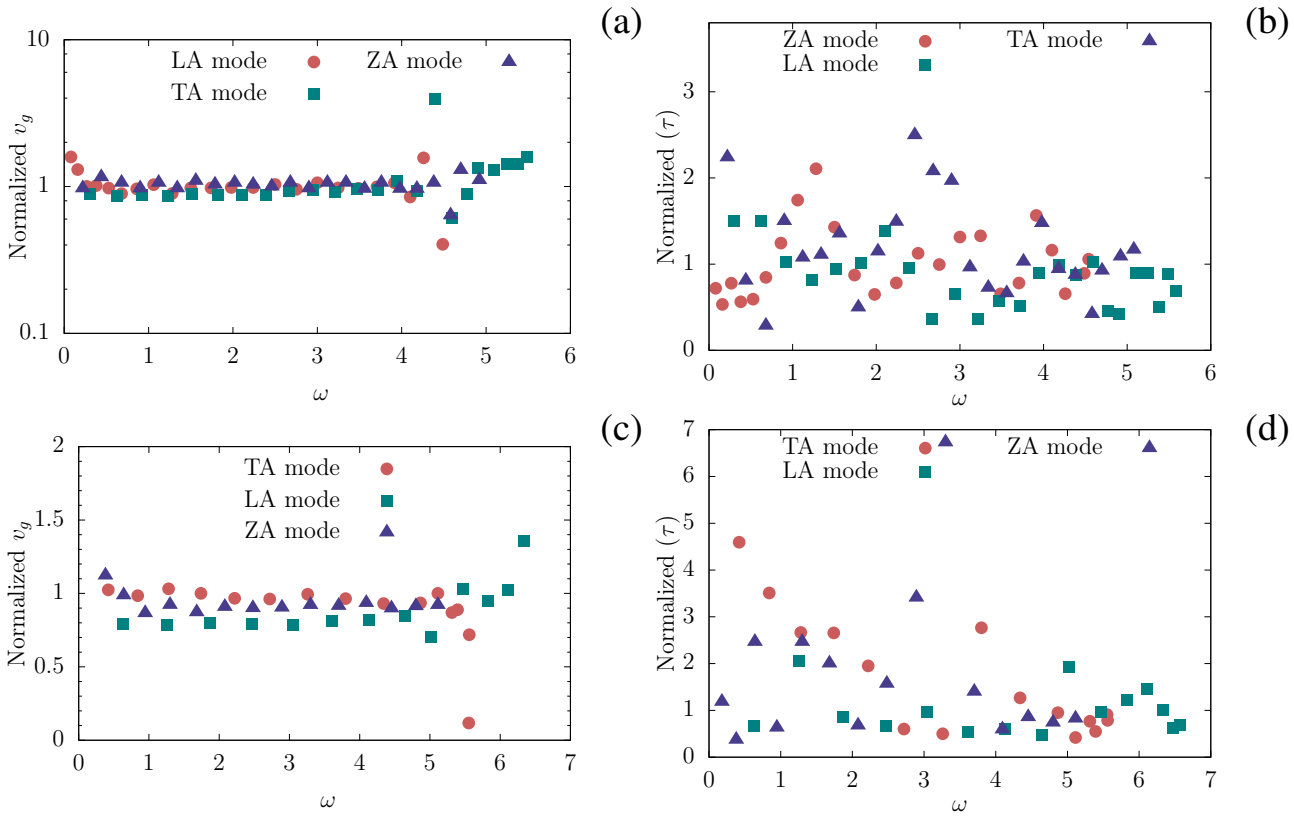

Figure 9: Normalized phonon group velocities of (a) MoS_2 (c) BP. Normalized phonon relaxation time for (b) MoS_2 (d) BP

Figures 8,9 represent the normalized phonon group velocities and relaxation time for graphene, h-BN, MoS_2 and BP. The normalized phonon properties (v_g, τ) are obtained by dividing the mode quantities at desired strain by their zero strain counterparts i.e, $v_{g,strain}/v_{g,zero-strain}$ and $\tau_{strain}/\tau_{zero-strain}$.

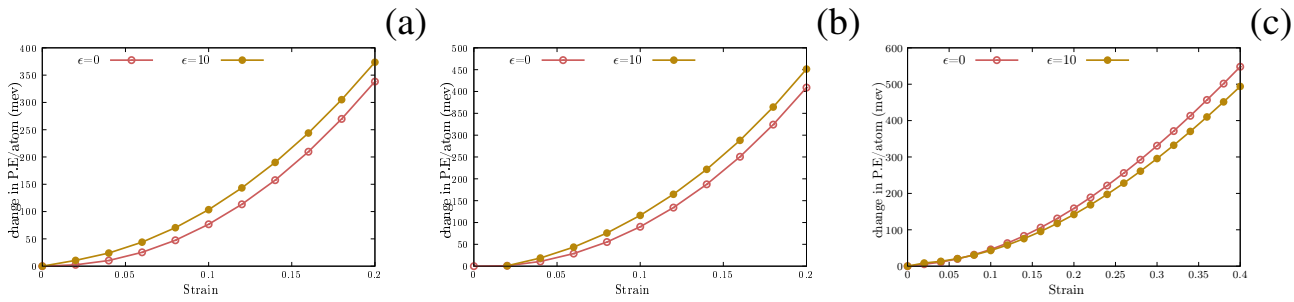

Figure 10: Energy-displacement curve of pristine and strained graphene along (a) zigzag (b) armchair and (c) out-of-plane direction

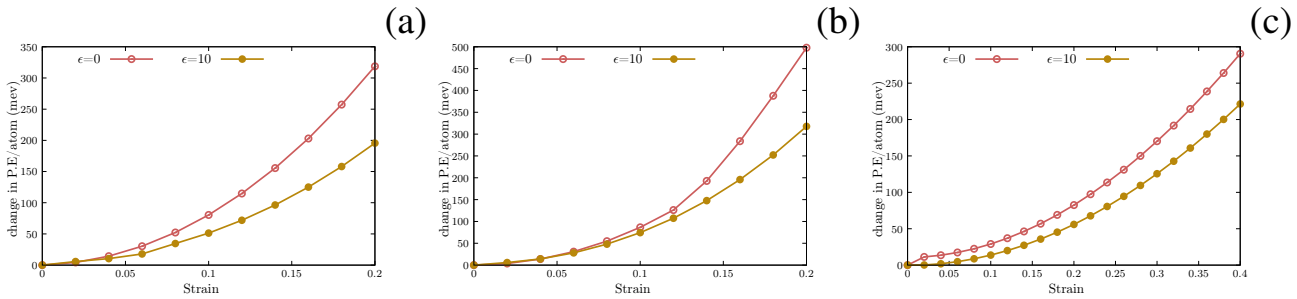

Figure 11: Energy-displacement curve of pristine and strained h-BN along (a) zigzag (b) armchair and (c) out-of-plane direction