Supplementary Information

Thermal transport in a defective pillared graphene network : Insights from equilibrium molecular dynamics simulation

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S1. Comparison of simulation results

To validate our simulation procedure, we conducted equilibrium molecular dynamics (EMD) simulations using the Green-Kubo formalism for a graphene nanoribbon measuring 10 $nm \times 1\ nm \times 0.34\ nm$ in dimension, as illustrated in Fig.S1. The chosen system dimensions were adopted from Ref.[S1] and [S2] to facilitate a comparison of the computed thermal conductivity. Initially, the system was thermally equilibrated at 300 K through a Nose-Hoover thermostat in the NVT ensemble, employing 3×10^5 time steps. Subsequently, the NVE ensemble was employed for 1×10^7 time steps to calculate the heat flux correlation function. The carbon-carbon interaction was modeled using an optimized Tersoff potential with a time step of 0.5 fs. Consistency was maintained in the simulation procedure, potential, and system dimensions, following Ref.[S1] and [S2]. The resulting thermal conductivities were compared and illustrated in Fig.S2. Notably, our computed thermal conductivity aligns well with the values reported in Ref.[S1] and [S2].

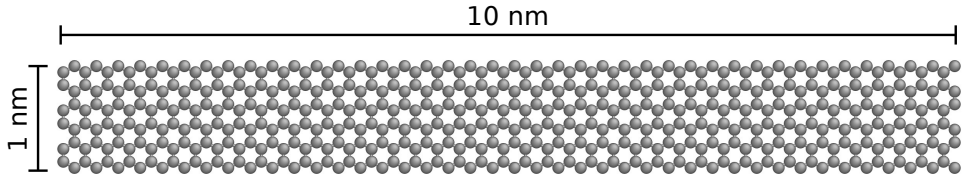


Figure S1: Graphene nanoribbon.

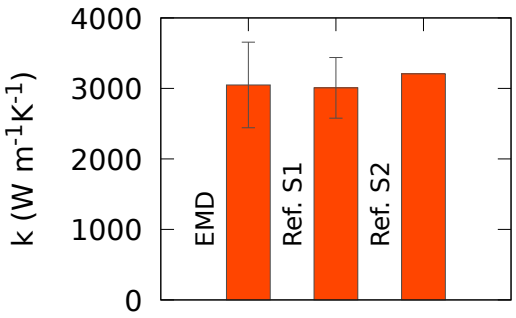


Figure S2: Thermal conductivity of graphene nanoribbon.

S2. Effect of system size on thermal conductivity

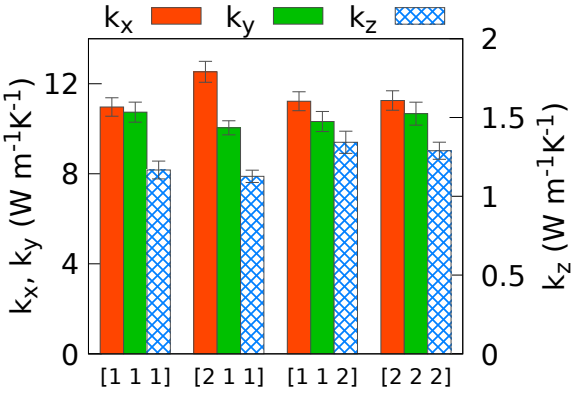
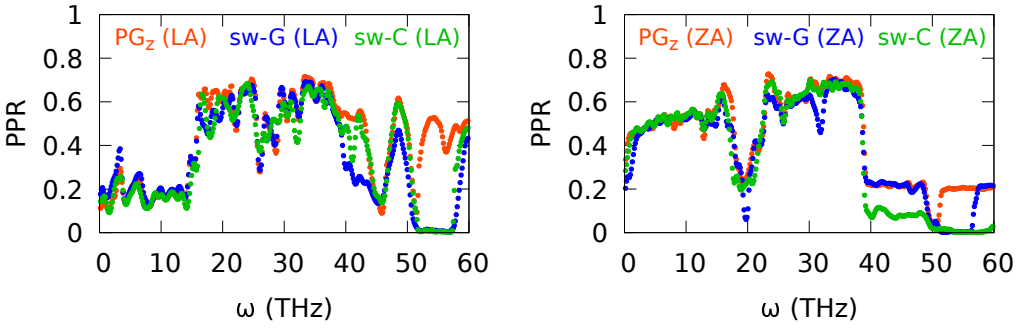


Figure S3: Thermal conductivity of a PG system with varying system dimensions. The values within the brackets [ ] indicate the number of unit cells considered for the analysis along the x, y and z directions, respectively.

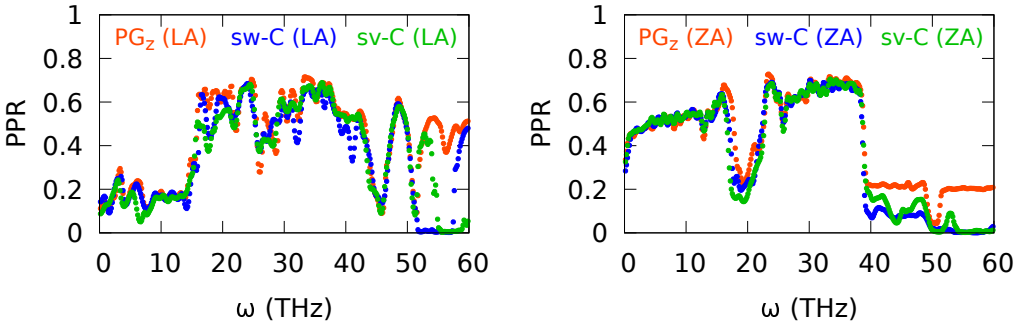
S3. Comparison of PPR to study the effect of defect location in PG_z configuration



(a) (b)

Figure S4: (a)-(b) Comparative analysis of phonon participation ratio in defect-free and defective PG_z configuration at LA and ZA phonon modes.

S4. Comparison of PPR to study the effect of defect type in PG_z configuration



(a) (b)

Figure S5: (a)-(b) Comparative analysis of phonon participation ratio in defect-free, sw-C, and sv-C PG_z configurations for LA and ZA phonon modes.

References

[S1] W. J. Evans, L. Hu, and P. Keblinski, "Thermal conductivity of graphene ribbons from equilibrium molecular dynamics: Effect of ribbon width, edge roughness, and hydrogen termination," *Applied Physics Letters*, vol. 96, no. 20, 2010.

[S2] A. I. Khan, I. A. Navid, M. Noshin, H. A. Uddin, F. F. Hossain, and S. Subrina, "Equilibrium molecular dynamics (md) simulation study of thermal conductivity of graphene nanoribbon: a comparative study on md potentials," *Electronics*, vol. 4, no. 4, pp. 1109–1124, 2015.