Supplementary information for

Thermal Transport Properties of Defective Graphene/Graphyne van der Waals Heterostructures Elucidated via Molecular Dynamics and Machine Learning

Jian Li, Jin Zhang*

School of Science, Harbin Institute of Technology, Shenzhen 518055, PR China

*Corresponding author. E-mail address: jinzhang@hit.edu.cn (J. Zhang).

Supplementary figures

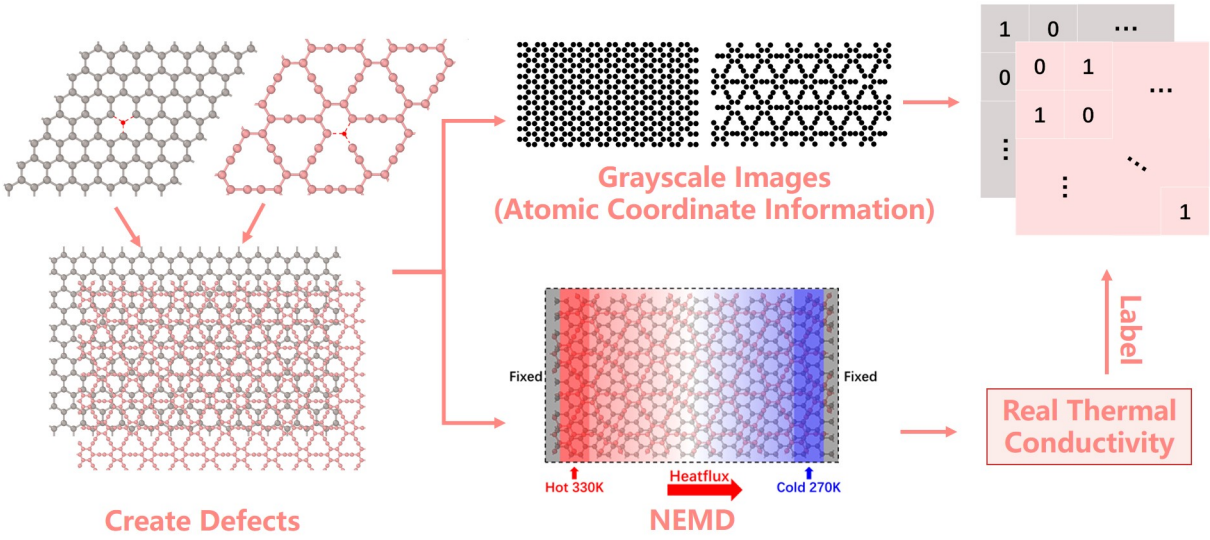

Fig. S1. The process of building the dataset.

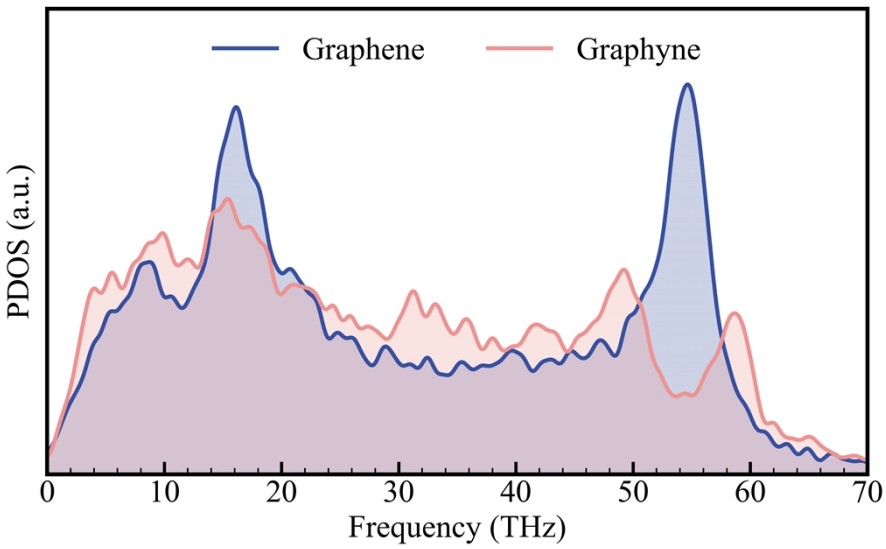

Fig. S2. The calculated phonon density of state (PDOS) of graphene and graphyne layers in pristine G/GY.

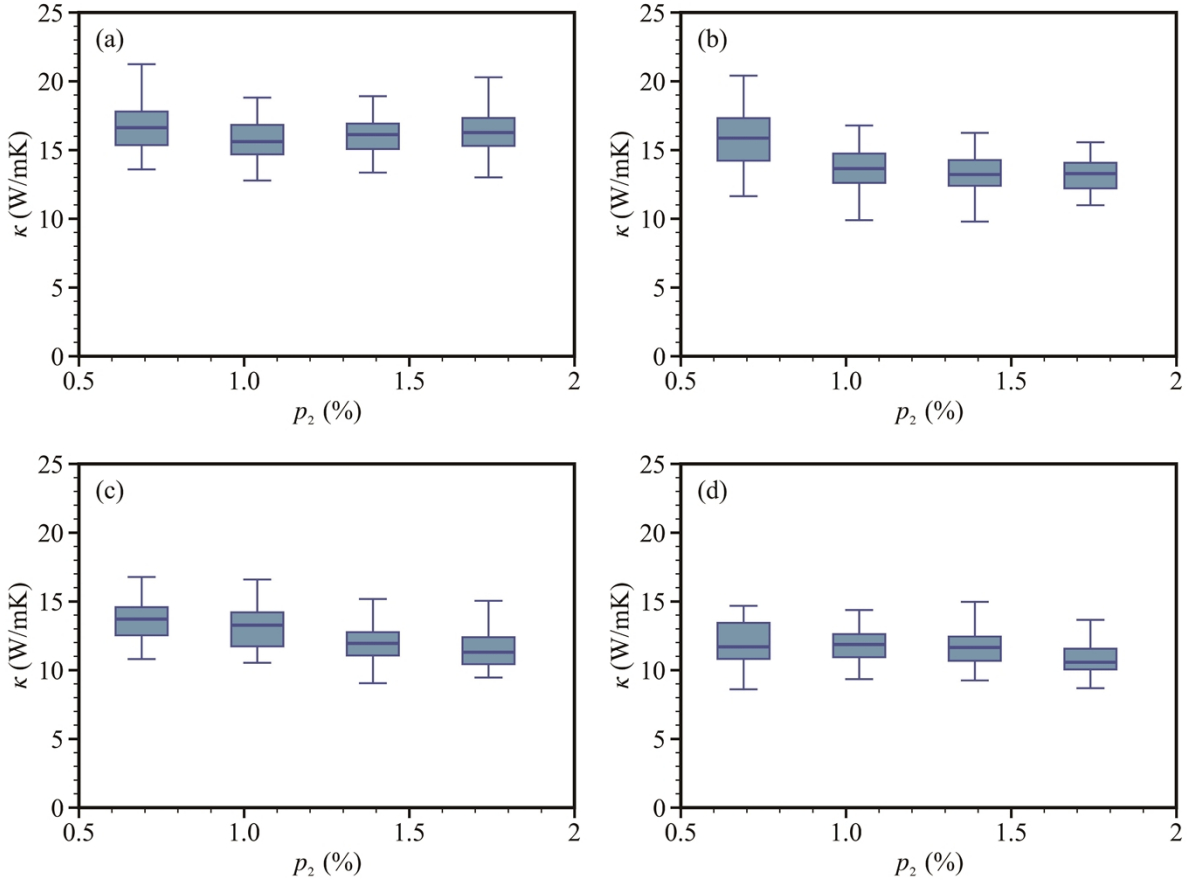

Fig. S3. Thermal conductivities of G/GY with various p_2 when p_1 is (a) 0.5%, (b) 1.0%, (c) 1.5% and (d) 2.0%.

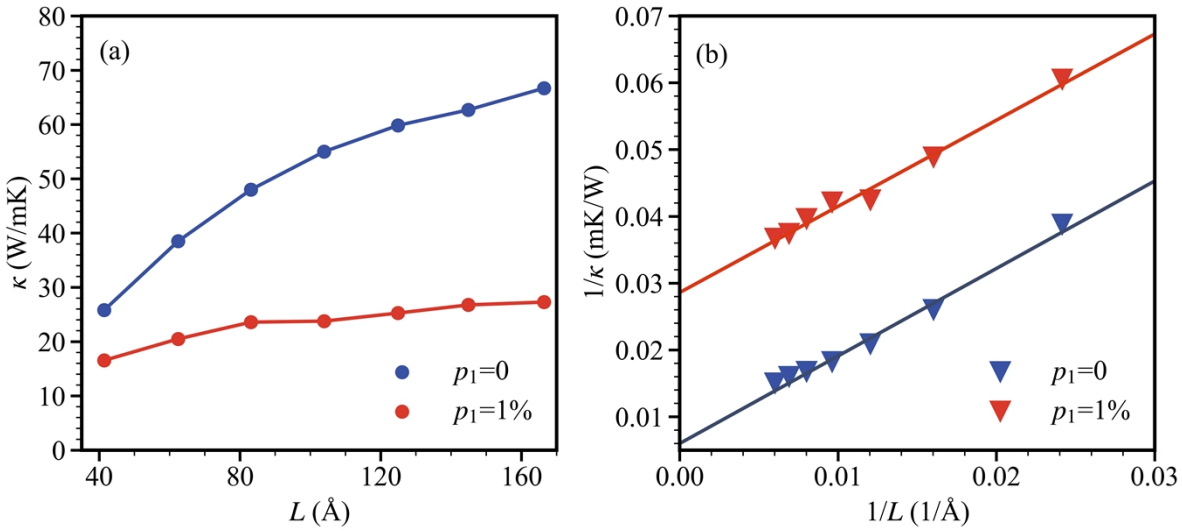

Fig. S4. (a) Thermal conductivities of pristine G/GY ($p_1 = 0$) and defective G/GY ($p_1 = 1\%$) with different lengths. (b) Relation between the inverse thermal conductivity and the inverse length of G/GY, which can be well fitted by the Matthiessen's rule (see the solid lines).

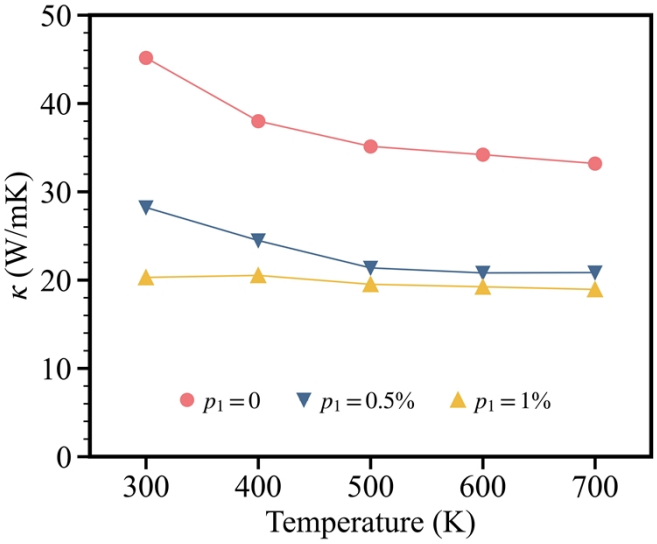

Fig. S5. Thermal conductivities of G/GY at different temperatures.

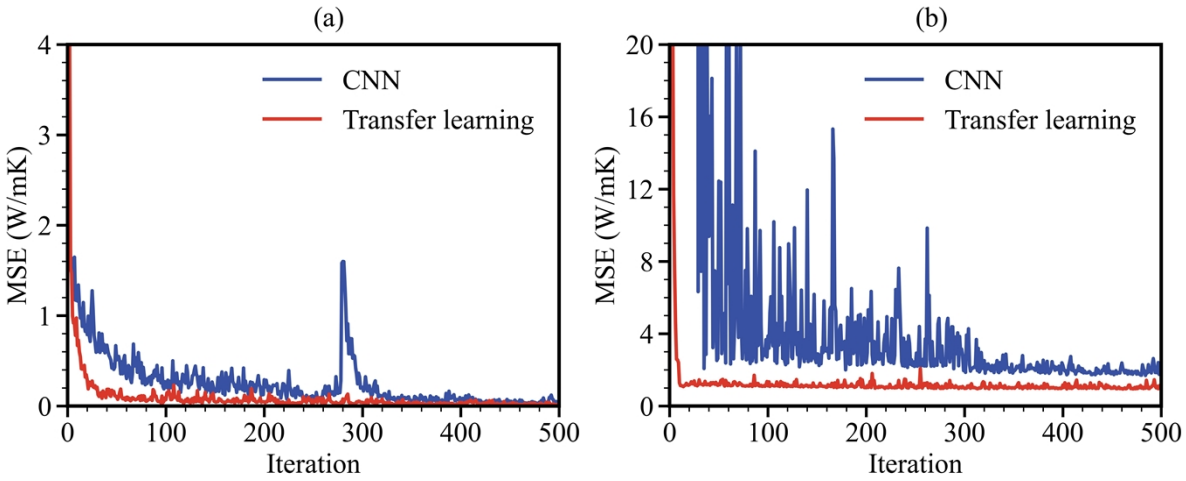

Fig. S6. Comparison of the MSE of CNN and transfer learning performed on (a) training set and (b) validation set.