

Supplementary Information for the article:

## Phonons and thermal conducting properties of borocarbonitride (BCN) nanosheets

Himanshu Chakraborty, Santosh Mogurampelly, Vivek K. Yadava, Umesh V. Waghmare and  
Michael L. Klein

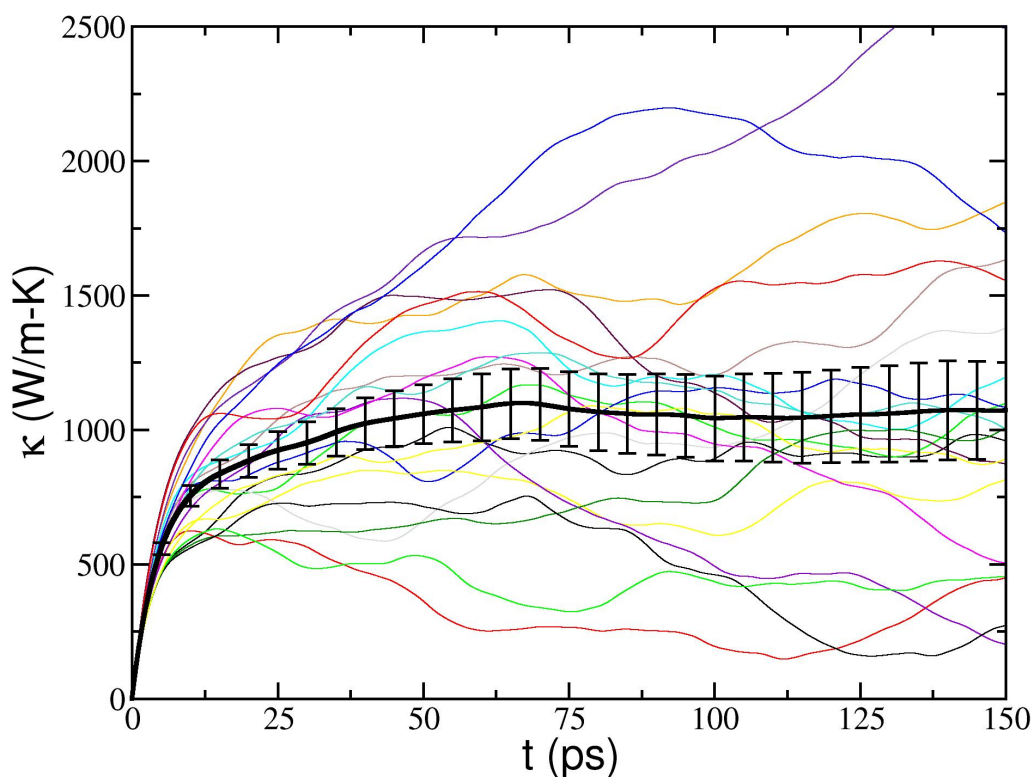


Fig. S1 Thermal conductivity of graphene monolayer as a function of upper time limit for the integration (see Eq. 2 of the main paper) calculated from 20 independent classical MD simulations. Black line corresponds to the average of the thermal conductivity from these simulations. The thermal conductivity is seen to approach a constant value after approximately 50 ps but, however, we chose 150 ps as the upper limit for the integration.

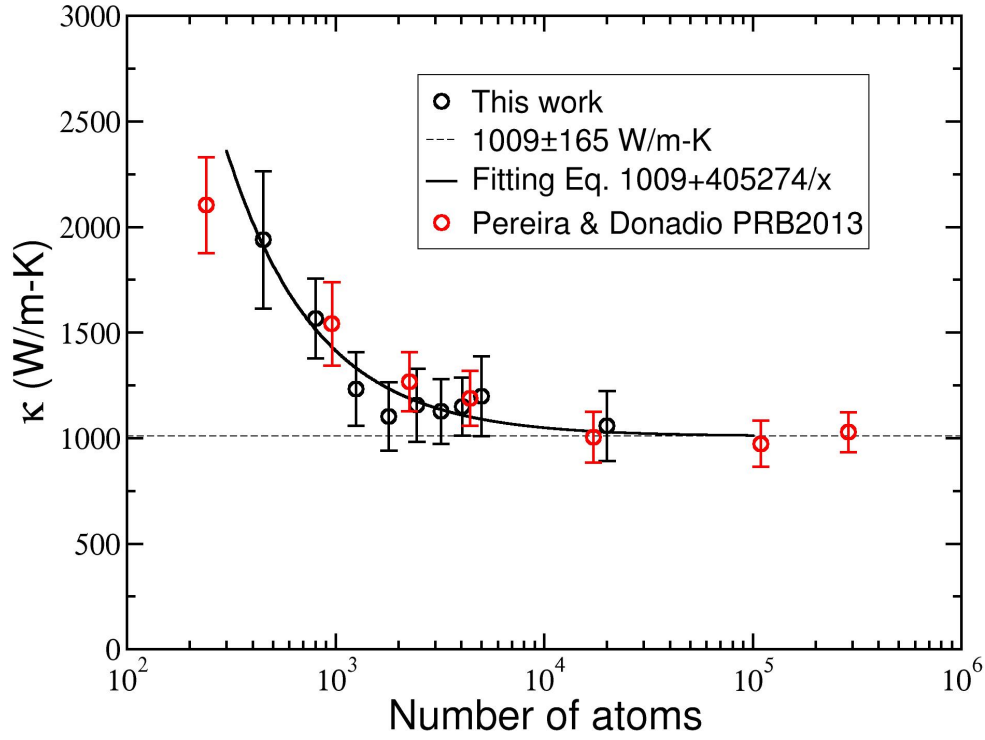


Fig. S2 Thermal conductivity of graphene monolayers as a function of the number of atoms (equivalently, the system size) calculated from classical MD simulations. Note that the thermal conductivity converges for system sizes of 20000 atoms or more, and the results presented in the main paper corresponds to such a big system (25.1 nm x 21.7 nm).

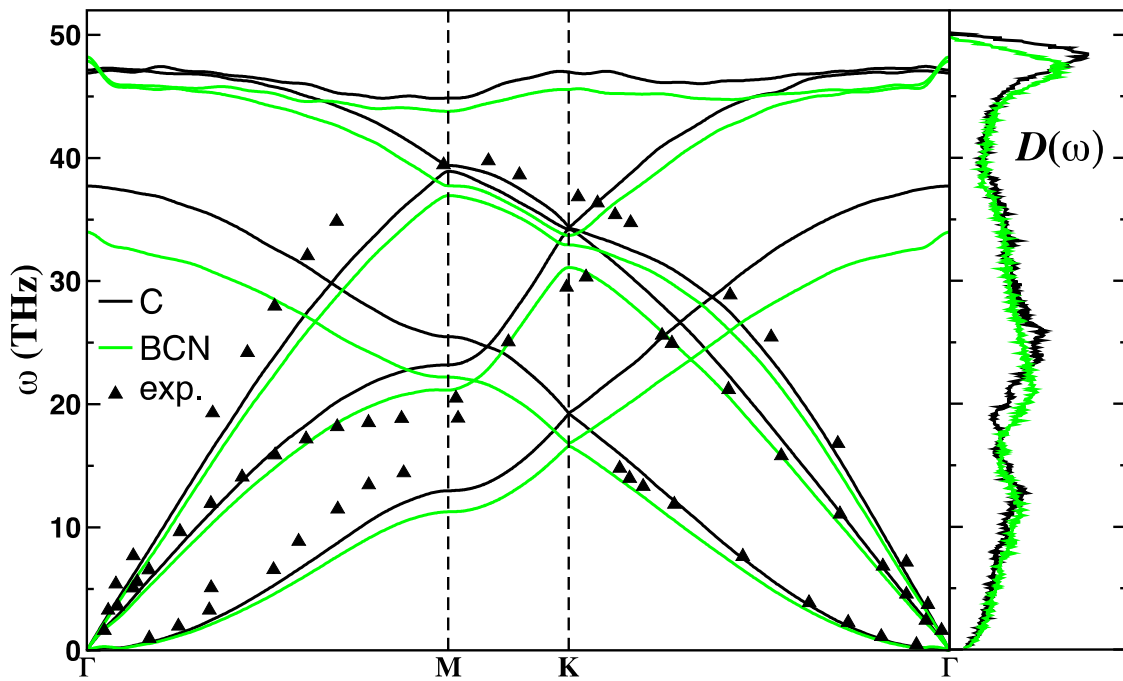


Fig. S3 Phonon dispersion curves for graphene and BCN monolayers and the respective density of states. The experimental data for graphene is shown for comparison.