ELECTRONIC SUPPLEMENTARY INFORMATION

Electronic, optical and thermoelectric properties of boron-doped Nitrogenated Holey Graphene

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I. B-DOPED NHG STRUCTURES BEFORE OPTIMIZATION

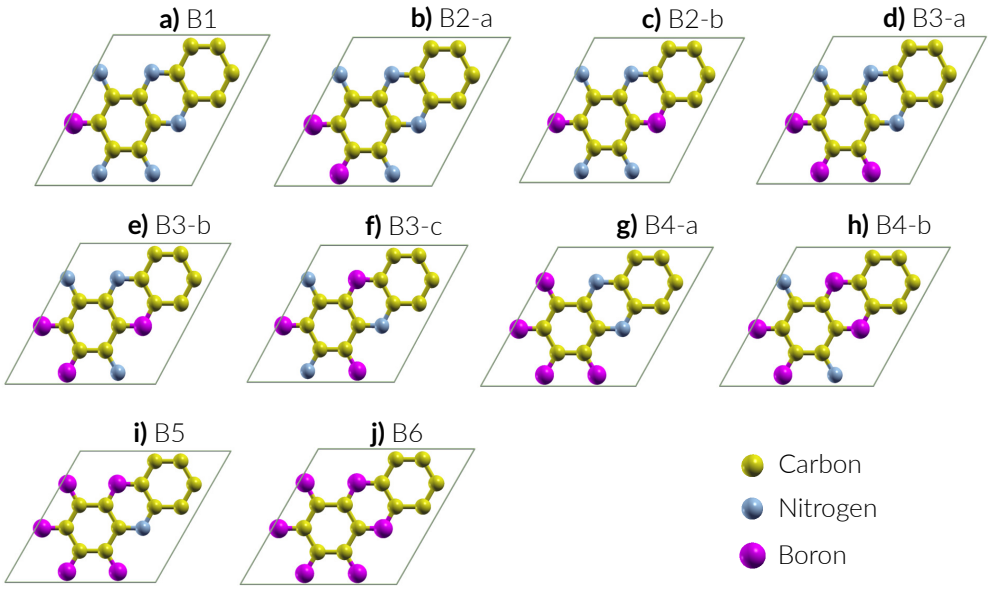

FIG. 1. Unit cell of the boron doped NHG monolayers. The number of boron substitutions ranges from 1 to 6.

II. LATTICE THERMAL CONDUCTIVITY CALCULATION

In general, the calculation of the lattice thermal conductivity with molecular dynamics simulations are somewhat size-dependent. However, starting from small systems it is possible to obtain the intrinsic (size-independent) thermal conductivity of a material adjusting the following expression to the data points

$$\kappa(L) = \kappa \left(1 + \frac{\Lambda}{L}\right)^{-1}, \tag{1}$$

where $\kappa(L)$ is the size-dependent conductivity and κ is the intrinsic quantity. Here, Λ presents an average phonon mean free path on the material. In the diffusive transport regime $L >> \Lambda$, and $\kappa(L) \approx \kappa$. The conductivities reported in the manuscript were obtained from the data in Fig. 2.

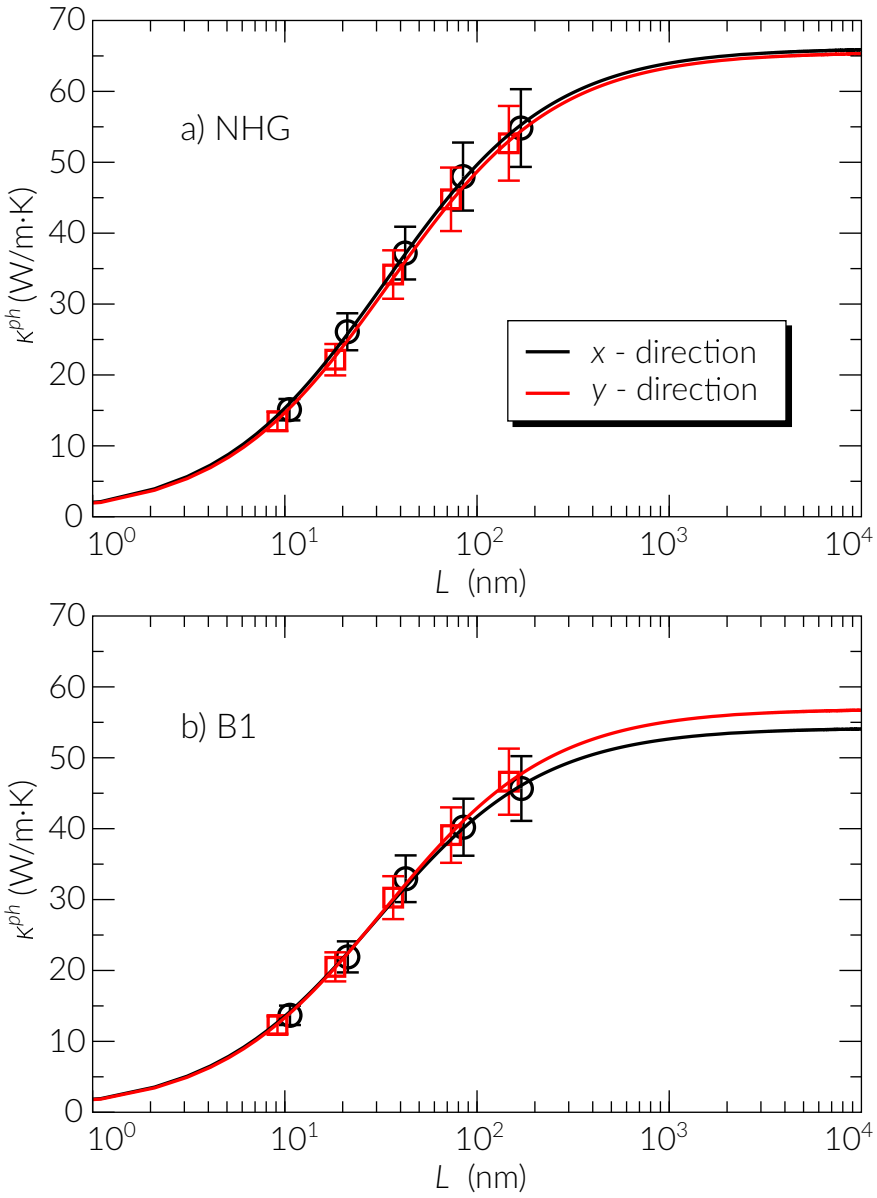

FIG. 2. Size dependence of the thermal conductivity obtained from molecular dynamics simulations.