ELECTRONIC SUPPLEMENTARY INFORMATION

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

Raphael M. Tromer,1,2,3,* A. Freitas,1 Isaac M. Felix,1 Bohayra Mortazavi,4 L. D. Machado,1 S. Azevedo,5 and Luiz Felipe C. Pereira1,6†

1Departamento de Física, Universidade Federal do Rio Grande do Norte, Natal, 59078-970, Brazil
2Applied Physics Department, State University of Campinas, Campinas, SP, 13083-970, Brazil
3Center for Computational Engineering and Sciences, State University of Campinas, Campinas, SP, 13083-970, Brazil
4Chair of Computational Science and Simulation Technology, Department of Mathematics and Physics, Leibniz Universität Hannover, Appelstrasse 11, 30157 Hannover, Germany.
5Departamento de Física, CCEN, Universidade Federal da Paraíba, João Pessoa, 58051-970, Brazil.
6Departamento de Física, Universidade Federal de Pernambuco, Recife, 50670-901, Brazil

∗tromer@fisica.ufrn.br
†pereira@fisica.ufrn.br
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

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

where \( \kappa(L) \) is the size-dependent conductivity and \( \kappa \) is the intrinsic quantity. Here, \( \Lambda \) 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.