Supplemental on-line EPAPS material for

Computational study of the thermal conductivity in defective carbon nanostructures

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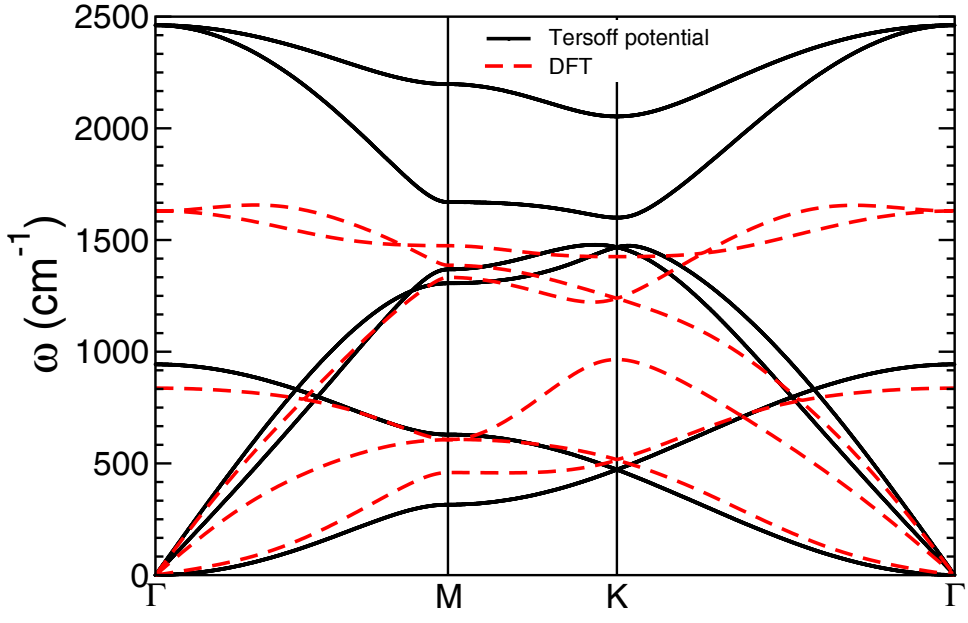

FIG. S1. (Color online) Vibration spectrum of graphene along high symmetry directions in the Brillouin zone obtained using the Tersoff potential (black solid lines) and *ab initio* density functional theory (DFT) calculations (red dashed lines).

Vibration spectra of graphene

To confirm the suitability of the Tersoff potential [1] for phonon-based thermal conductivity calculations, we determined the vibration spectrum of graphite using this approach and present the results in Fig. S1. For the sake of comparison, we generated the same vibration spectrum using *ab initio* density functional calculations as implemented in the SIESTA code [2,3] and present them in the same figure. The SIESTA calculations used the Ceperley-Alder exchange-correlation functional[4] as parameterized by Perdew and Zunger[5] and described the interaction between valence electrons and ions by norm-conserving pseudopotentials[6] with separable non-local operators[7]. Atomic orbitals with double-ζ polarization were used to expand the electron wave functions with an energy cutoff of 100 Ry for the real-space mesh representation of the charge density.

We find that the Tersoff potential provides an adequate description of the acoustic modes, but generally overestimates the frequency of the optical modes by up to 50%.

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[1] J. Tersoff, Phys. Rev. Lett. **61**, 2879 (1988).
[2] D. Sanchez-Portal, P. Ordejon, E. Artacho, J. M. Soler, Int. J. Quantum Chem. **65**, 453 (1997).
[3] J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon, D. Sanchez-Portal, J. Phys. Cond. Matter **14**, 2745 (2002).
[4] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
[5] J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[6] N. Troullier and J. L. Martins, Phys. Rev. B **43**, 1993 (1991).
[7] L. Kleinman and D. M. Bylander, Phys. Rev. Lett. **48**, 1425 (1982).