
Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths

Giorgia Fugallo¹, Andrea Cepellotti², Lorenzo Paulatto³, Michele Lazzeri³, Nicola Marzari², Francesco Mauri³

1) *European Theoretical Spectroscopy Facility, Laboratoire des Solides Irradiés, École Polytechnique, 91128 Palaiseau cedex, France*

2) *École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland*

3) *CNRS/ IMPMC, Université Pierre et Marie Curie, 4 place Jussieu, F-75252 Paris, France*

Corresponding author: Giorgia Fugallo (fugallo@theory.polytechnique.fr)

I will present a complete characterization of the thermal conductivity of graphite, graphene and related compounds, solving exactly [1] the Boltzmann transport equation (BTE) for phonons in the framework of density functional perturbation theory. For graphite, the results are found to be in excellent agreement with experiments and 1 order of magnitude larger than what found by solving the BTE in the standard relaxation time approximation. For graphene, a meaningful value of intrinsic thermal conductivity at room temperature can be obtained only for sample sizes of the order of 1 mm, something not considered previously [2]. This unusual requirement is because collective phonon excitations, and not single phonons, are the main heat carriers in these materials [2,3]; these excitations are characterized by mean free paths of the order of hundreds of micrometers. As a result i) the thermal conductivity is high but does not diverge in infinitely large systems and ii) the Fourier's law becomes questionable in typical sample size.

[1] G. Fugallo, M. Lazzeri, L. Paulatto, and F. Mauri, *Phys. Rev. B* 88, 045430 (2013).

[2] G. Fugallo, A. Cepellotti, L. Paulatto, M. Lazzeri, N. Marzari, and F. Mauri, *Nano Letters* 14, 6109 (2014)

[3] A. Cepellotti, G. Fugallo, L. Paulatto, M. Lazzeri, F. Mauri, and N. Marzari, *Nature Comm.* 6, 6400 (2015)

