International Workshop *Disordered Systems: From Localization to Thermalization and Topology*
3 -7 September 2018, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon, Korea

Quantum Size Effect in Phonon Thermal Transport in Graphene

Nica Jane Ferrer, Cristine Villagonzalo
National Institute of Physics, University of the Philippines Diliman
Quezon City, Philippines

The National Institute of Physics
University of the Philippines Diliman

NIP Photo: http://www.nip.upd.edu.ph (Dr. Percival Almoro)
Travel map : http://www.sunjinhan.blogspot.com

The Philippines:
Quick Facts

100,980,000 Population (2015 census)
(Median age: 24.1 yrs old)

7,107 Islands

2,299 Higher Education Institutions
(as of April 2013)

1,643 Private HEI
110 State Universities & Colleges
~20 with Physics programs

Population & island data from: www.gov.ph
HEI data: www.ched.gov.ph
MAP: www.madbookings.com

2016

Philippines' Physicists'

0.000125%
=
There is **one (1)**
physicist
for every
800,000 Filipinos.

Filipino physicists & linkages needed!

Philippines' Status of Theoretical Physics:

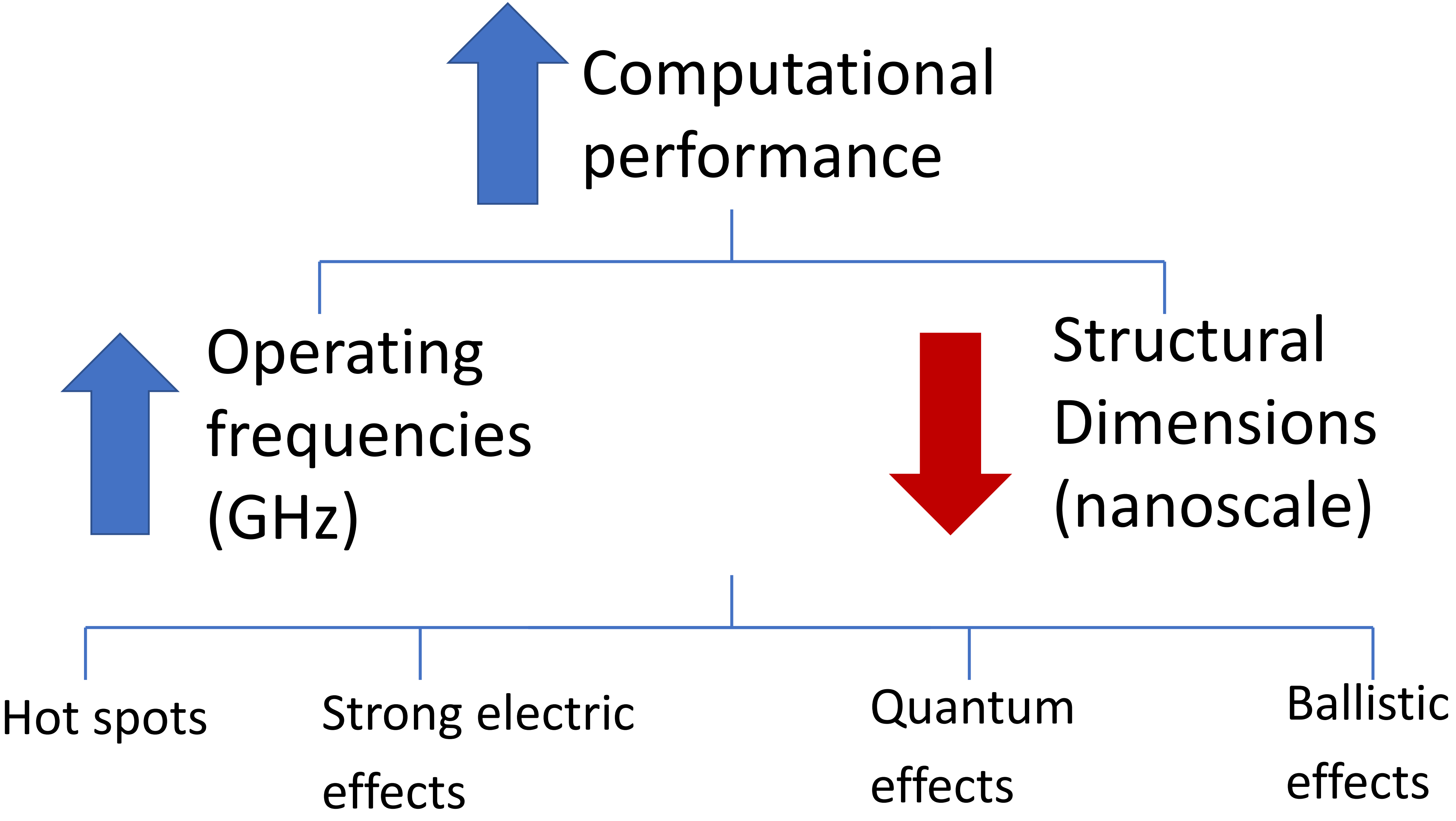
0.0000433468%
=
There is **one (1)**
theoretical physicist
for every
2,306,977 Filipinos.

Filipino physicists & linkages needed!

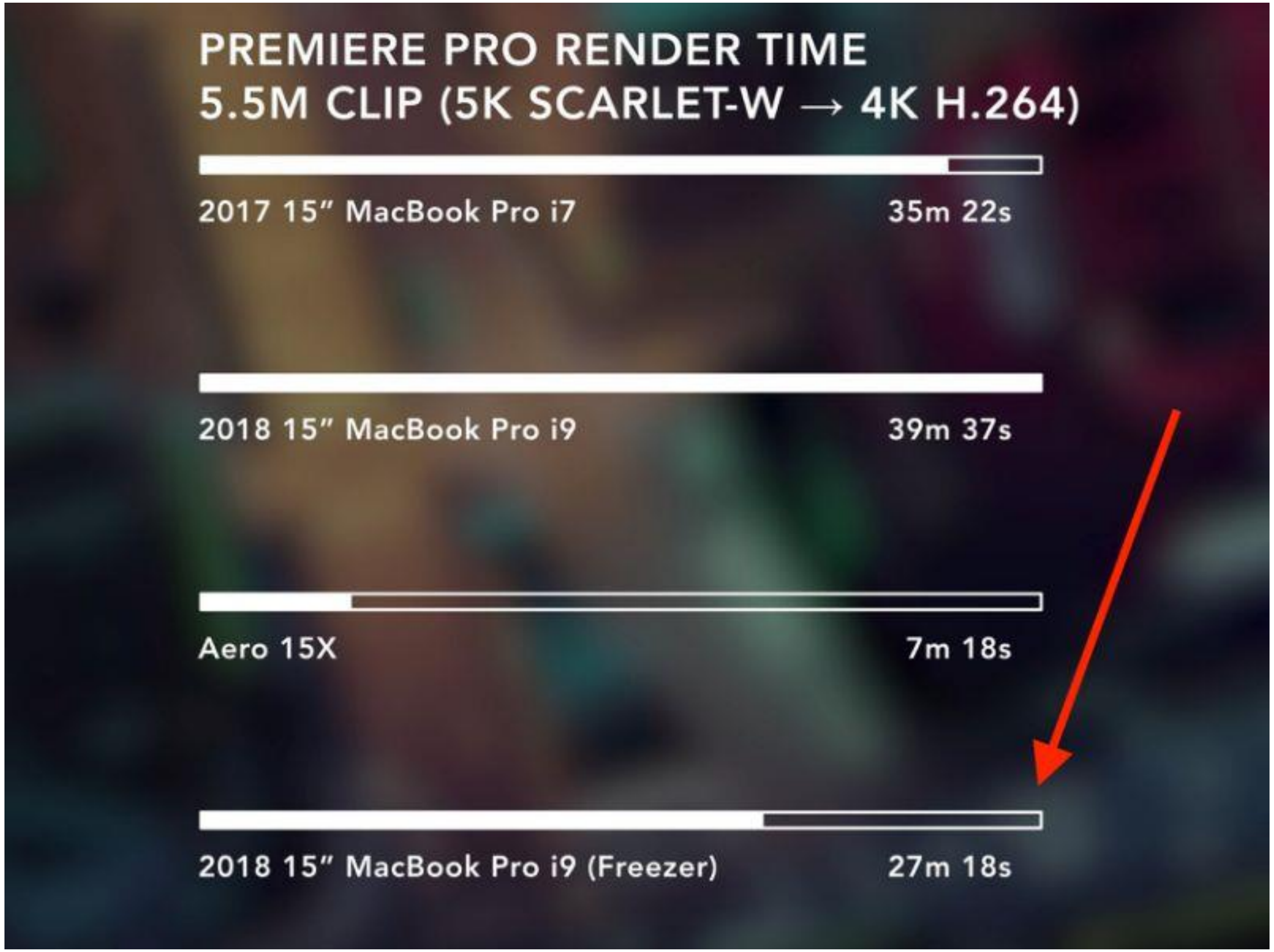
Overview

- **Motivation**
  - Thermal Throttling
  - Current Literature **on phonons in graphene**
- **The Method**
  - **NEGF**
- **Ballistic thermal transport in a graphene junction**
- **Summary & Conclusions**

Issues


Computational performance
Operating frequencies (GHz)
Structural Dimensions (nanoscale)
Hot spots
Strong electric effects
Quantum effects
Ballistic effects

Thermal Throttling



David Lee, Dave2D Youtube channel (2018)

Fourier's Law

Heat flux in the *z*-direction:

$$J_Q = -\kappa \frac{dT}{dz}$$

$$\kappa = \sigma \frac{l}{A}$$

Bulk lattice (at 300 K)	κ (W/mK)
silicon	140
natural diamond	2270
purified diamond	3450
graphite*	≈ 1500 – 2000
graphene	≈ 1500 – 4600

*Basal plane thermal conductivity

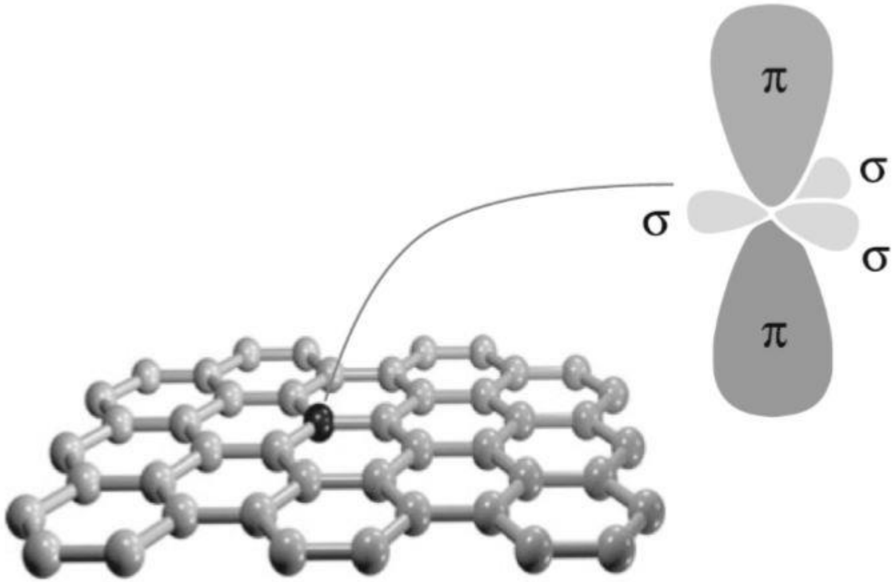
Data: A.L. Moore and L. Shi, *Materials Today* (2014)

Thermal conductivity

$$\kappa = \kappa_e + \kappa_l$$

dominant in metals

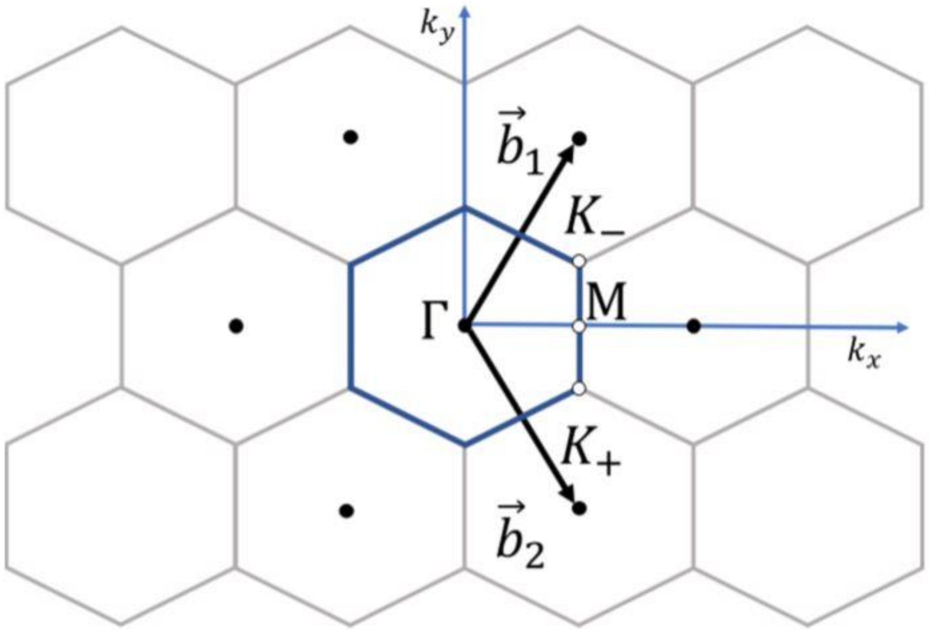
dominant in semiconductors & insulators

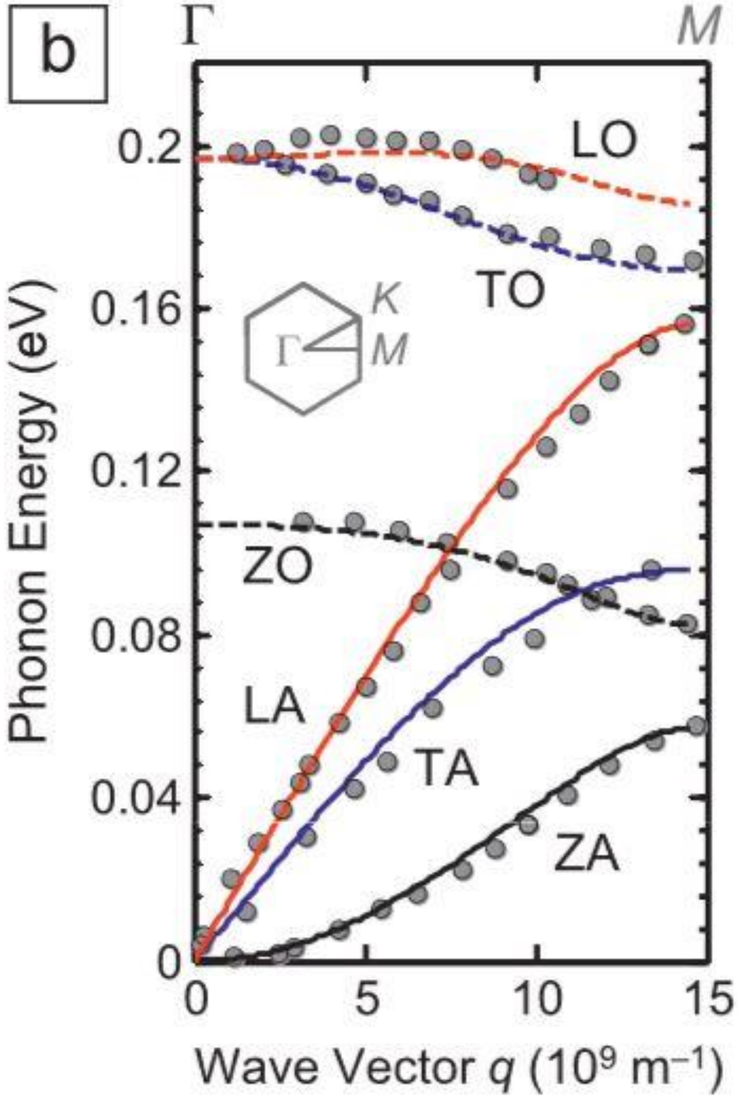


In graphene, electronic contribution is less than 1% at RT.
(S. Ghosh, *et al.*, APL 2008)

Graphene bonds: D. Van Tuan (Springer, 2016)

Phonon Spectrum





Phonon Spectra:
E. Pop, V. Varshney, A.K. Roy, *MRS Bulletin* 37 (2012) 1273

APPLIED PHYSICS LETTERS **92**, 151911 (2008)

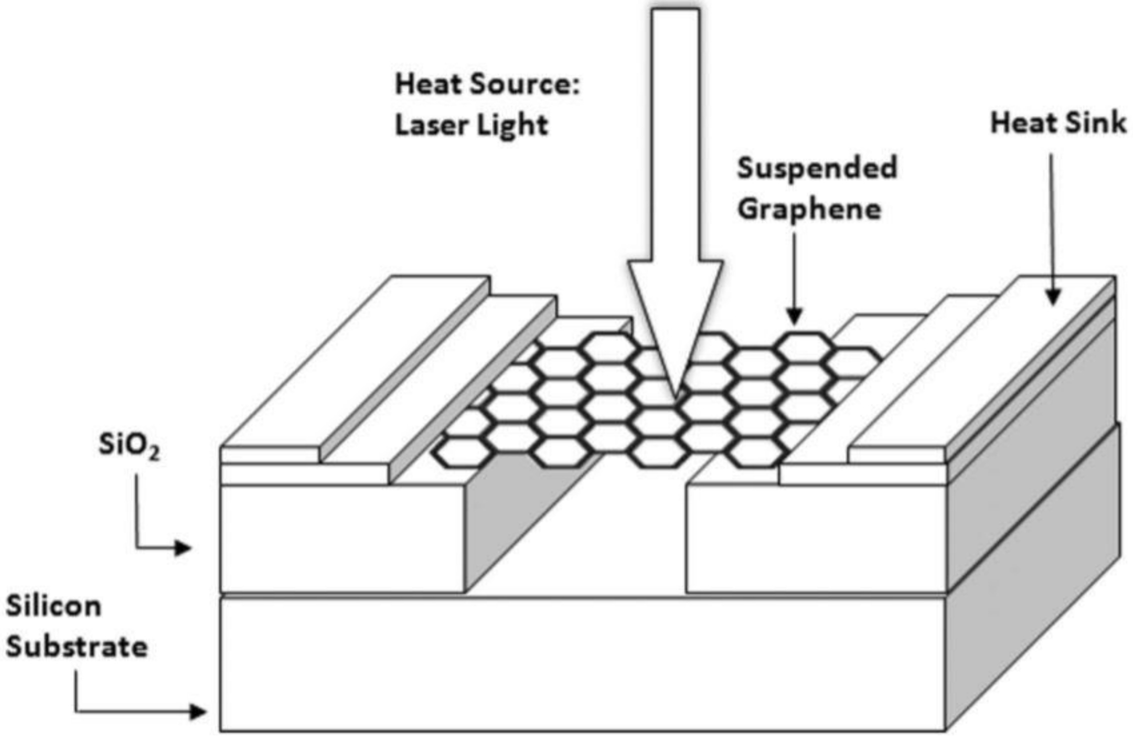
Extremely high thermal conductivity of graphene: Prospects for thermal management applications in nanoelectronic circuits

S. Ghosh,[1] I. Calizo,[1] D. Teweldebrhan,[1] E. P. Pokatilov,[1,a)] D. L. Nika,[1,a)] A. A. Balandin,[1,b)] W. Bao,[2] F. Miao,[2] and C. N. Lau[2]
[1]*Nano-Device Laboratory, Department of Electrical Engineering, University of California-Riverside, Riverside, California 92521, USA*
[2]*Department of Physics and Astronomy, University of California-Riverside, Riverside, California 92521 USA*

(Received 26 February 2008; accepted 18 March 2008; published online 16 April 2008)

The authors reported on investigation of the thermal conductivity of graphene suspended across trenches in Si/SiO_2 wafer. The measurements were performed using a noncontact technique based on micro-Raman spectroscopy. The amount of power dissipated in graphene and corresponding temperature rise were determined from the spectral position and integrated intensity of graphene's G mode. The extremely high thermal conductivity in the range of $\sim 3080-5150$ W/m K and phonon mean free path of ~ 775 nm near room temperature were extracted for a set of graphene flakes. The obtained results suggest graphene's applications as thermal management material in future nanoelectronic circuits. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2907977]

Suspended Graphene



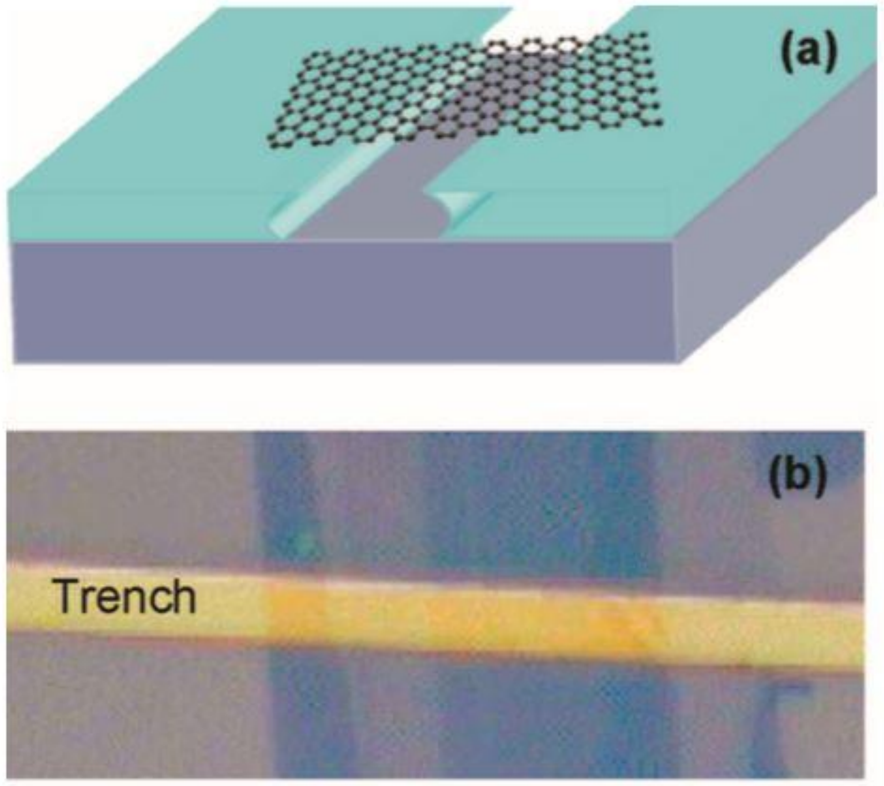
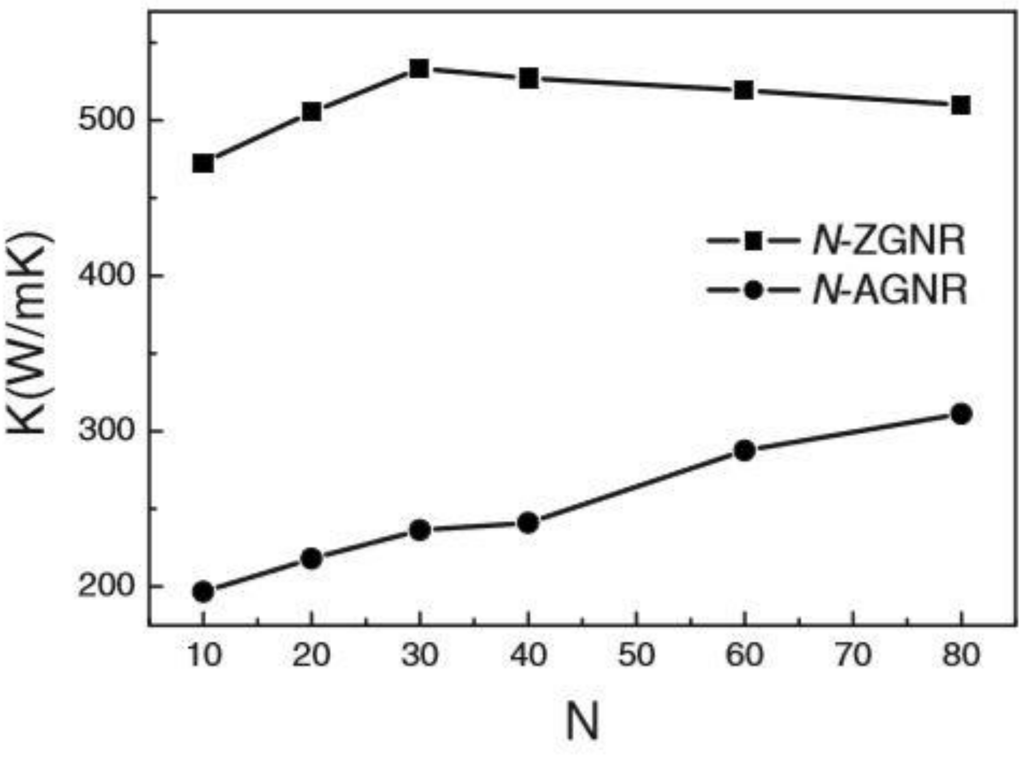
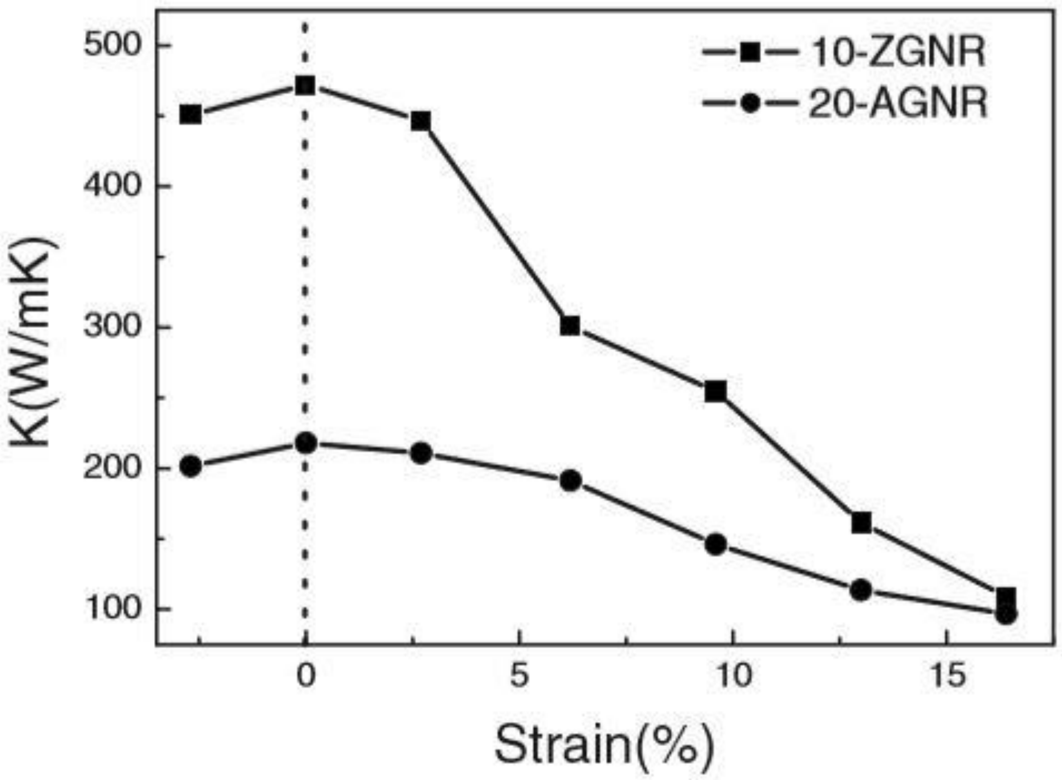


Image from: A.A. Balandin et al., *Fullerenes, Nanotubes & Carbon Nanostructures* 18 (2010) 474

Image from: S. Ghosh et al., *Appl Phys Lett* 92 (2008) 151911

GNR as a function of length and strain

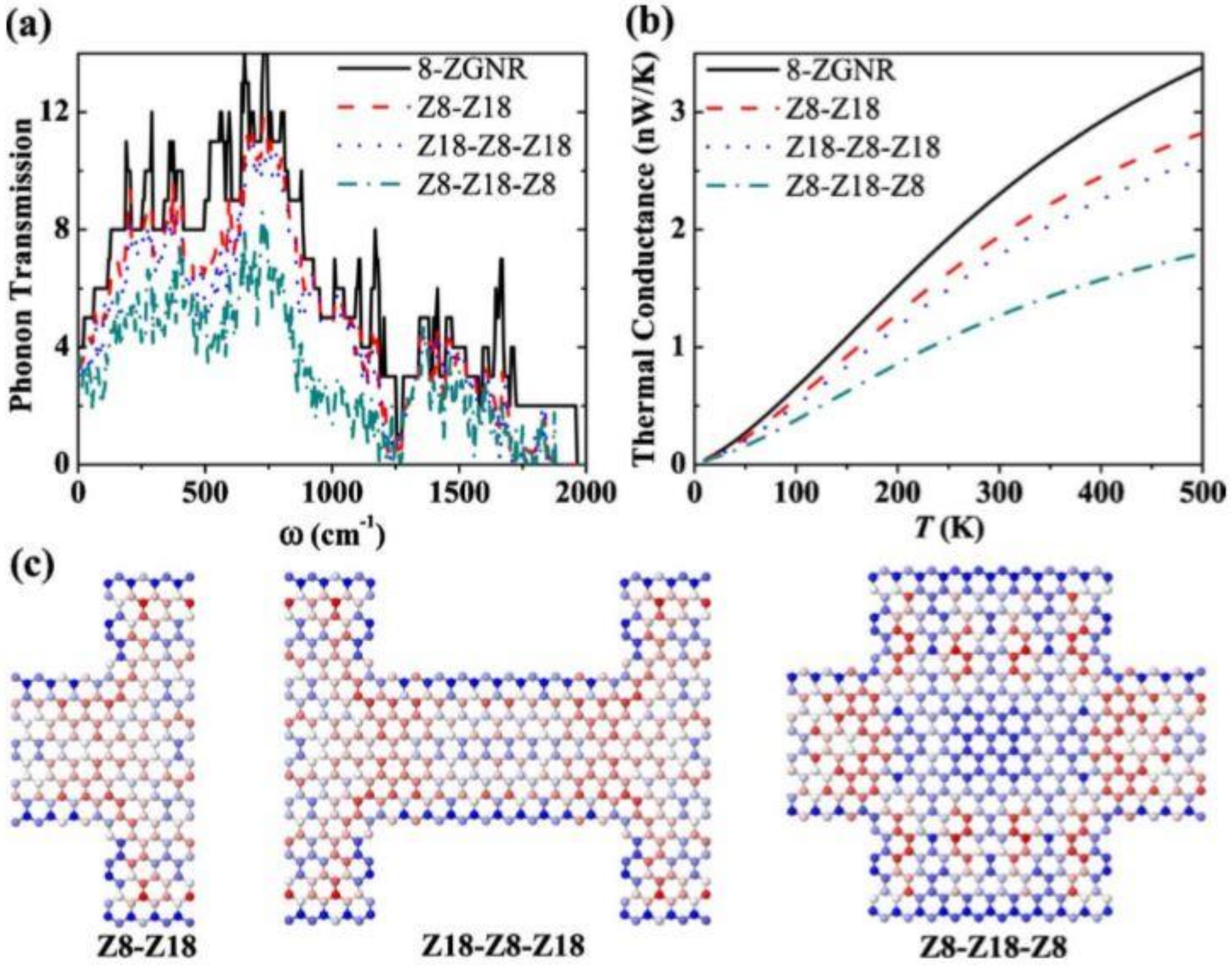




$\Delta T = 20$ K, unstrained length 11 nm

Z. Guo, D. Zhang & X.-G. Gong, *Appl Phys Lett* 95 (2009) 163103

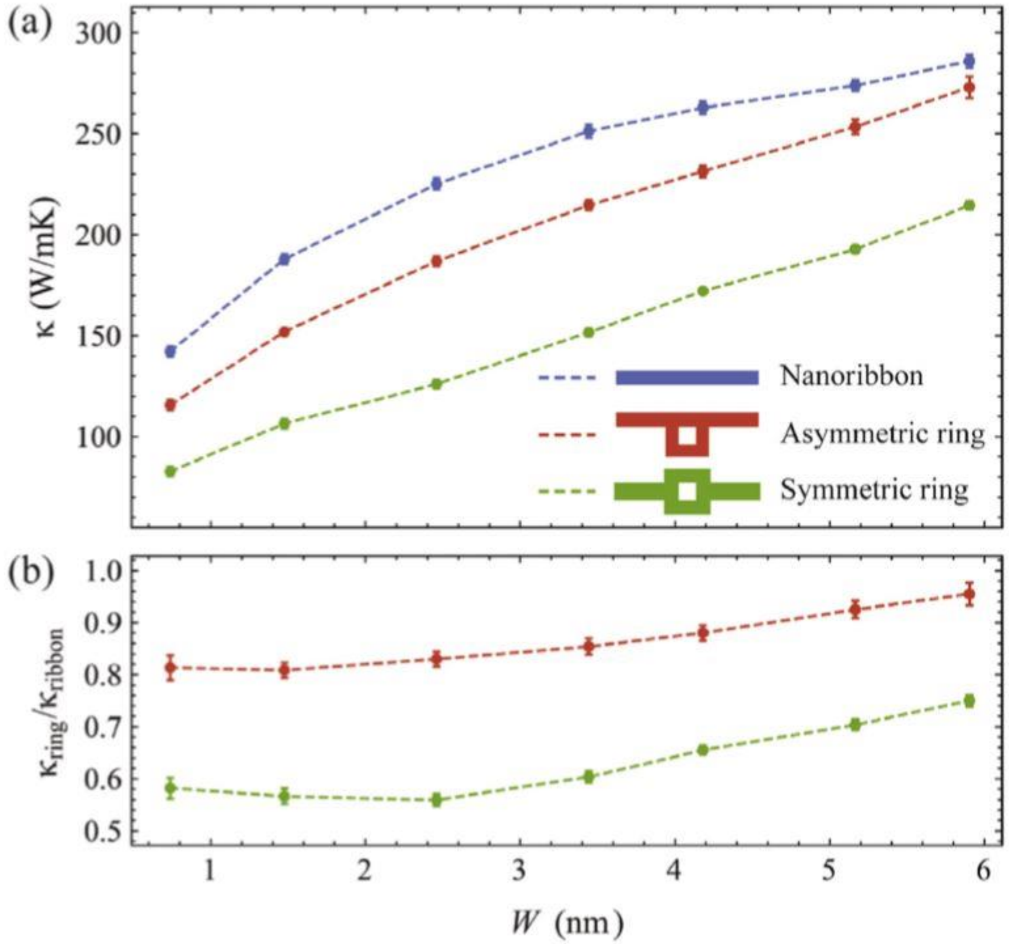
Graphene Nanodevices

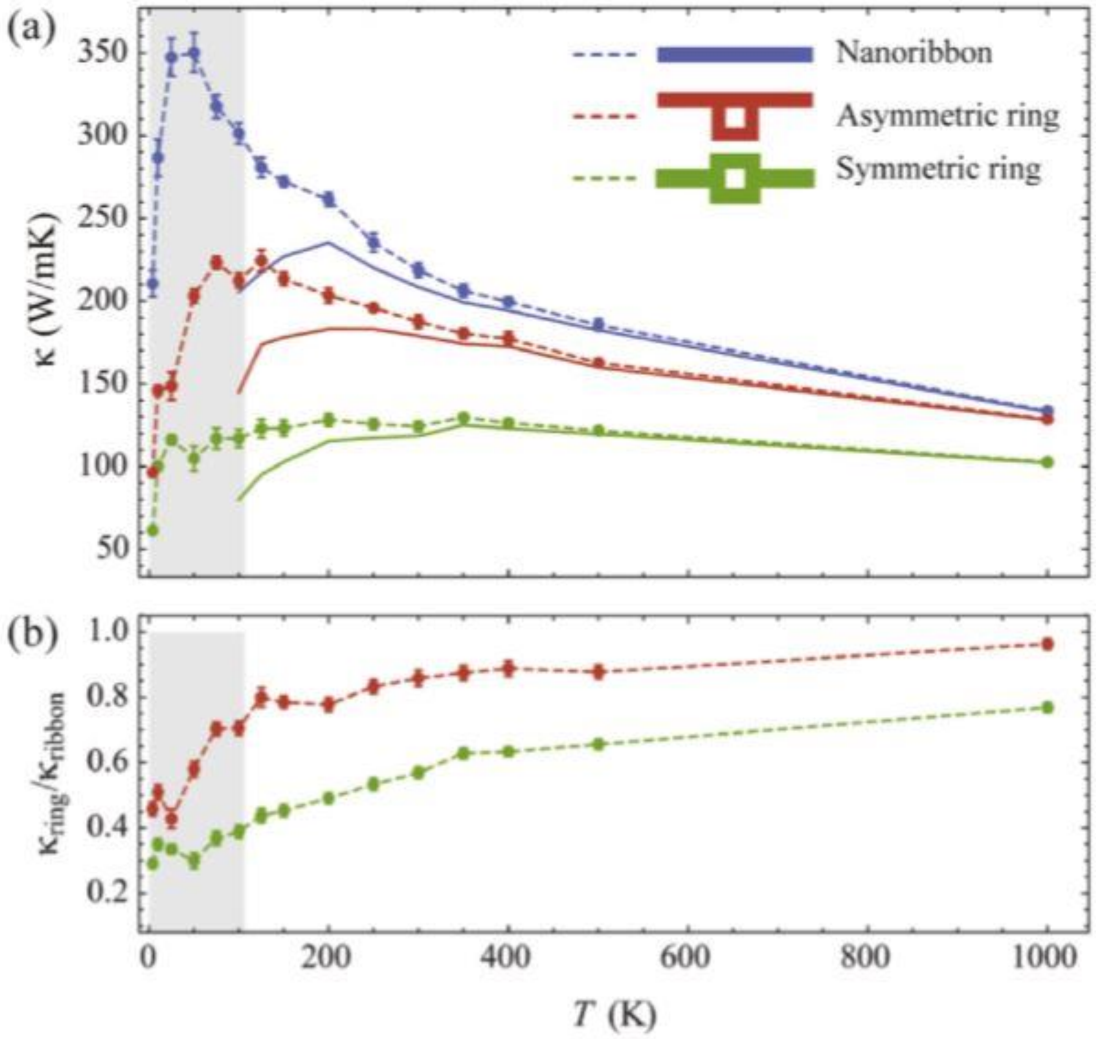


Y. Xu, X. Chen, J.-S. Wang, B.-L. Gu and W. Duan, *Phys. Rev. B* 81 (2010) 195425

Armchair GNR

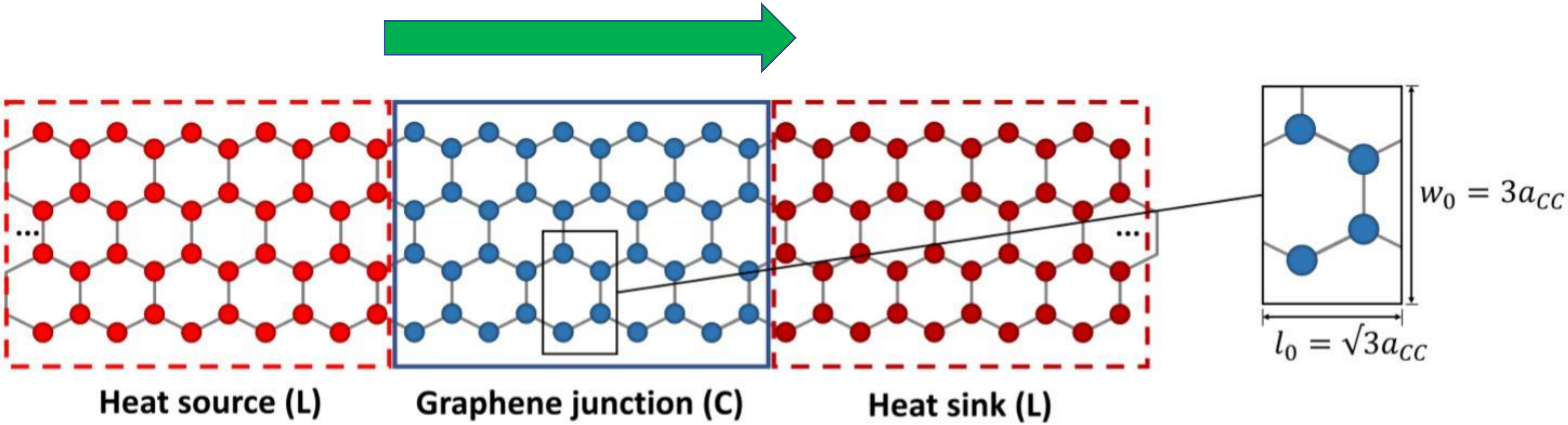
T = 300 K, Ls = 25.4 nm





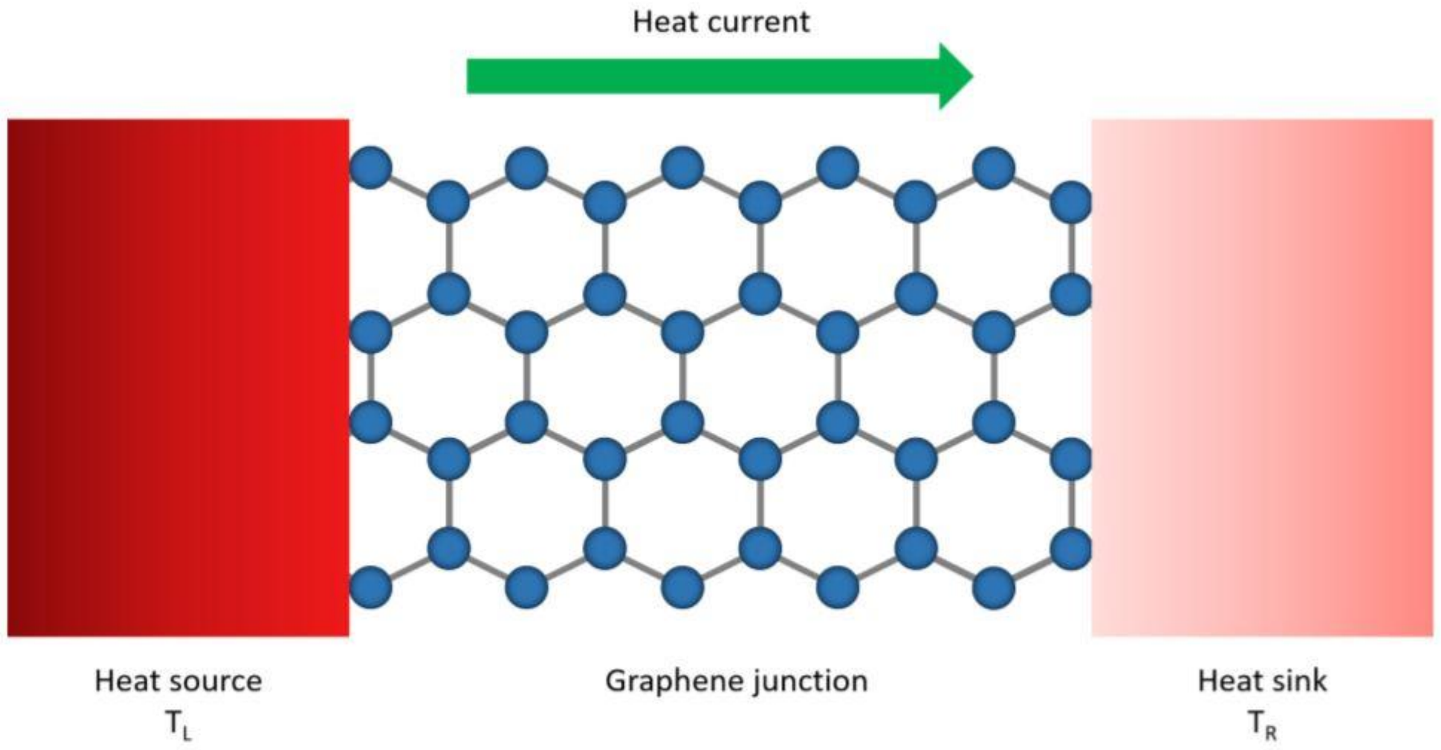
M. Saiz-Bretín, A.V. Maleyshev, F. Domínguez-Adame, D. Quigley and R.A. Römer, *Carbon* 127 (2018) 64

The Model: A Graphene Junction



$$L_{\mathrm{C}} \ll l_{\mathrm{mfp}}$$

Heat current



Landauer Formula:

$$I = \frac{1}{2\Pi}\int_0^\infty d\omega\ \hbar\omega\ \Xi(\omega)\ (f_L - f_R)$$

Thermal Conductance

$$\sigma(T) = \lim_{T_L \to T, T_R \to T} \frac{I}{T_L - T_R}$$

$\Delta T \ll T_L, T_R$

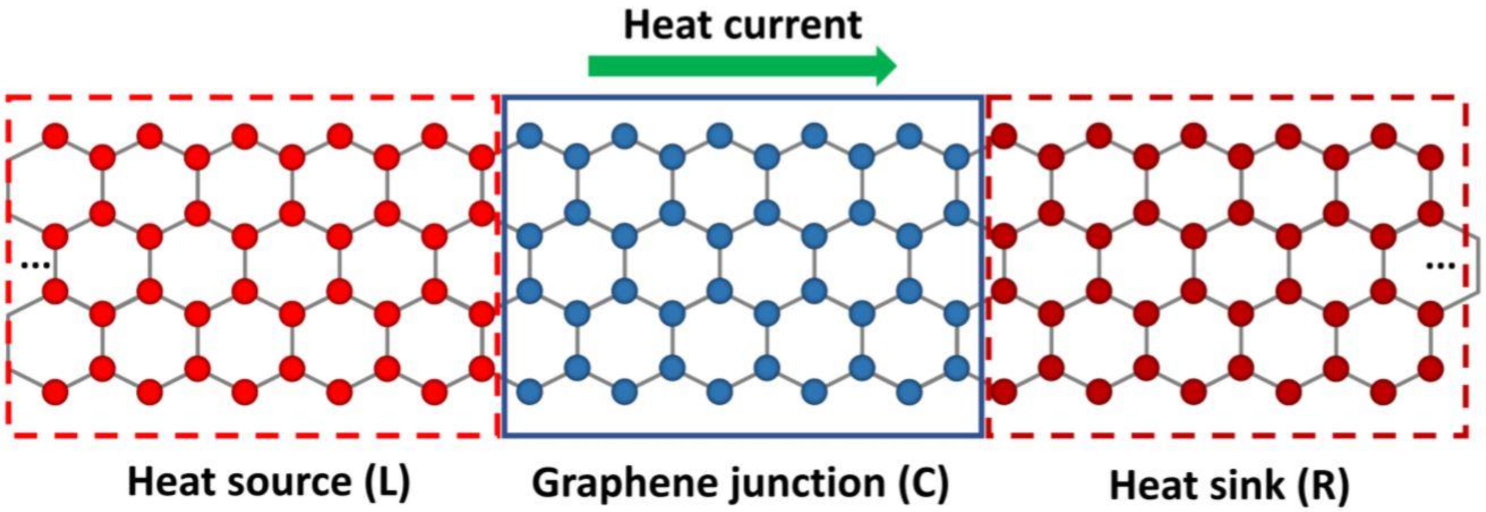
$$\sigma(T) = \frac{1}{2\Pi} \int_0^\infty d\omega \frac{\hbar^2 \omega^2}{k_B T^2} \underbrace{\Xi(\omega)} \frac{e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2}$$

The Hamiltonian

$$H = \sum_{\alpha=L,C,R} H_\alpha + (u^L)^T V^{LC} u^C + (u^C)^T V^{CR} u^R + V_n$$

$$H_\alpha = \frac{1}{2}\left[(\dot{u}^\alpha)^T \dot{u}^\alpha\right] + \frac{1}{2}\left[(u^\alpha)^T K^\alpha u^\alpha\right]$$

The NEGF Method

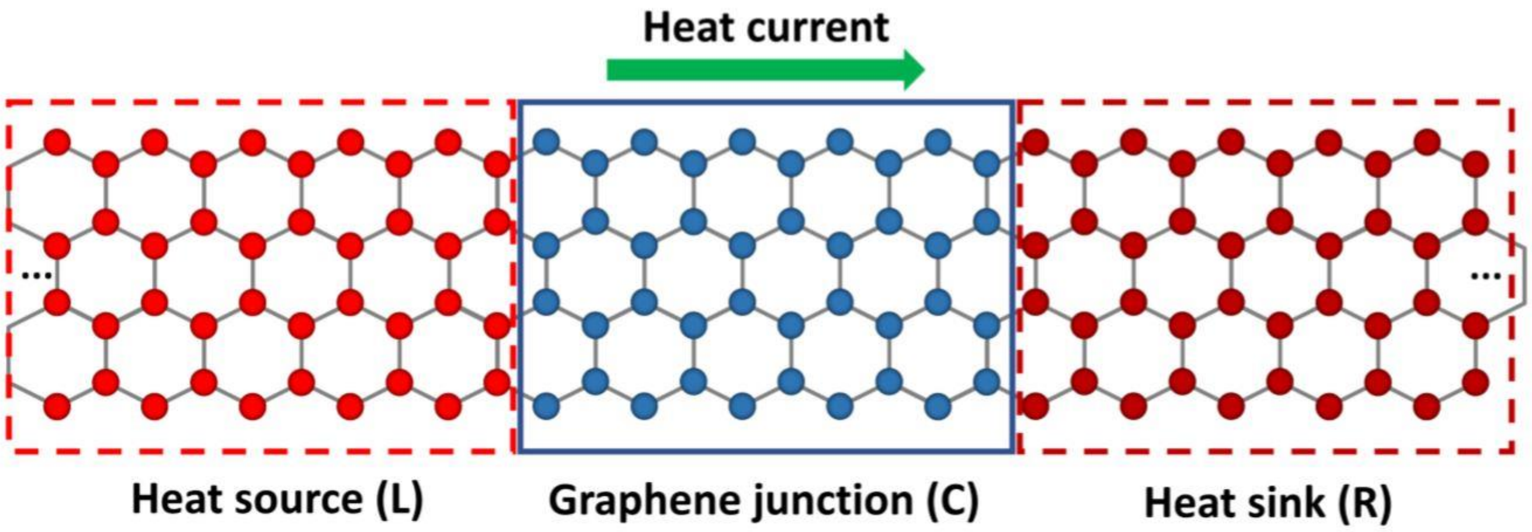


$$K = \begin{pmatrix} K^L & V^{LC} & 0 \\ V^{CL} & K^C & V^{CR} \\ 0 & V^{RC} & K^R \end{pmatrix}$$

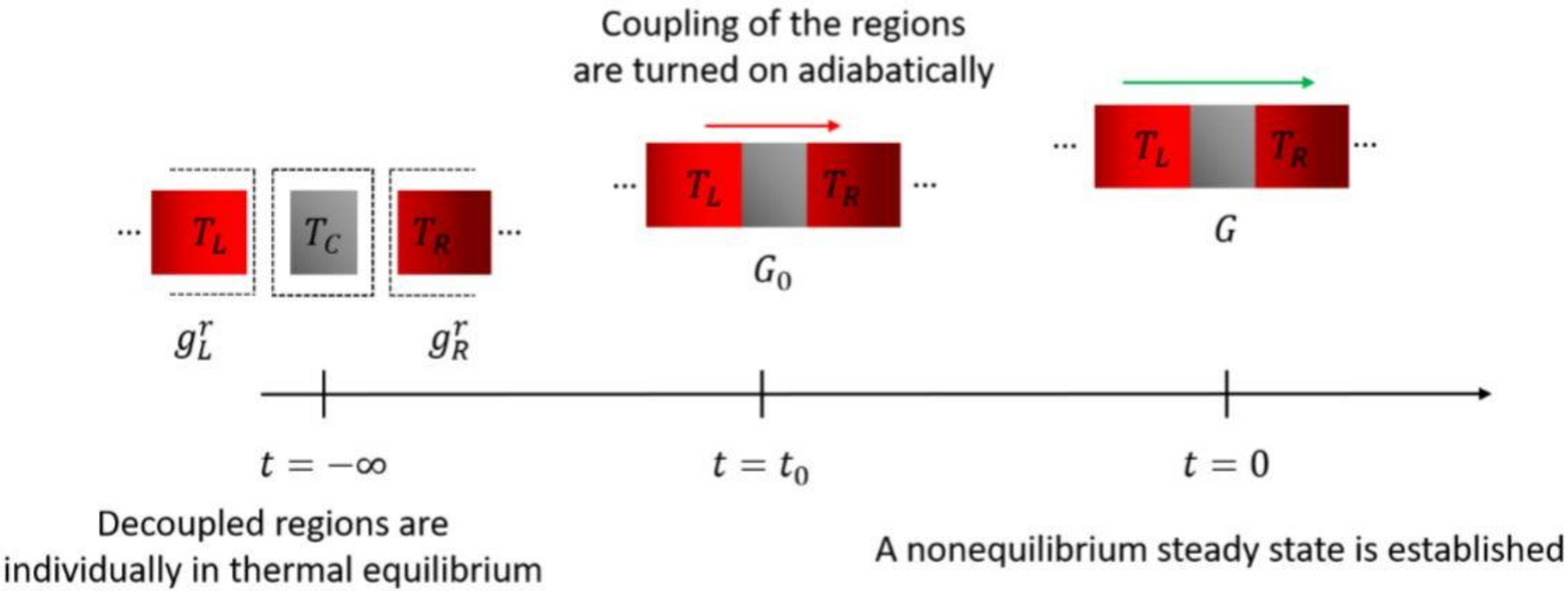
Caroli Formula

$$\Xi(\omega) = Tr\left[G_C^r(\omega)\Gamma_L(\omega)G_C^a(\omega)\Gamma_R(\omega)\right]$$

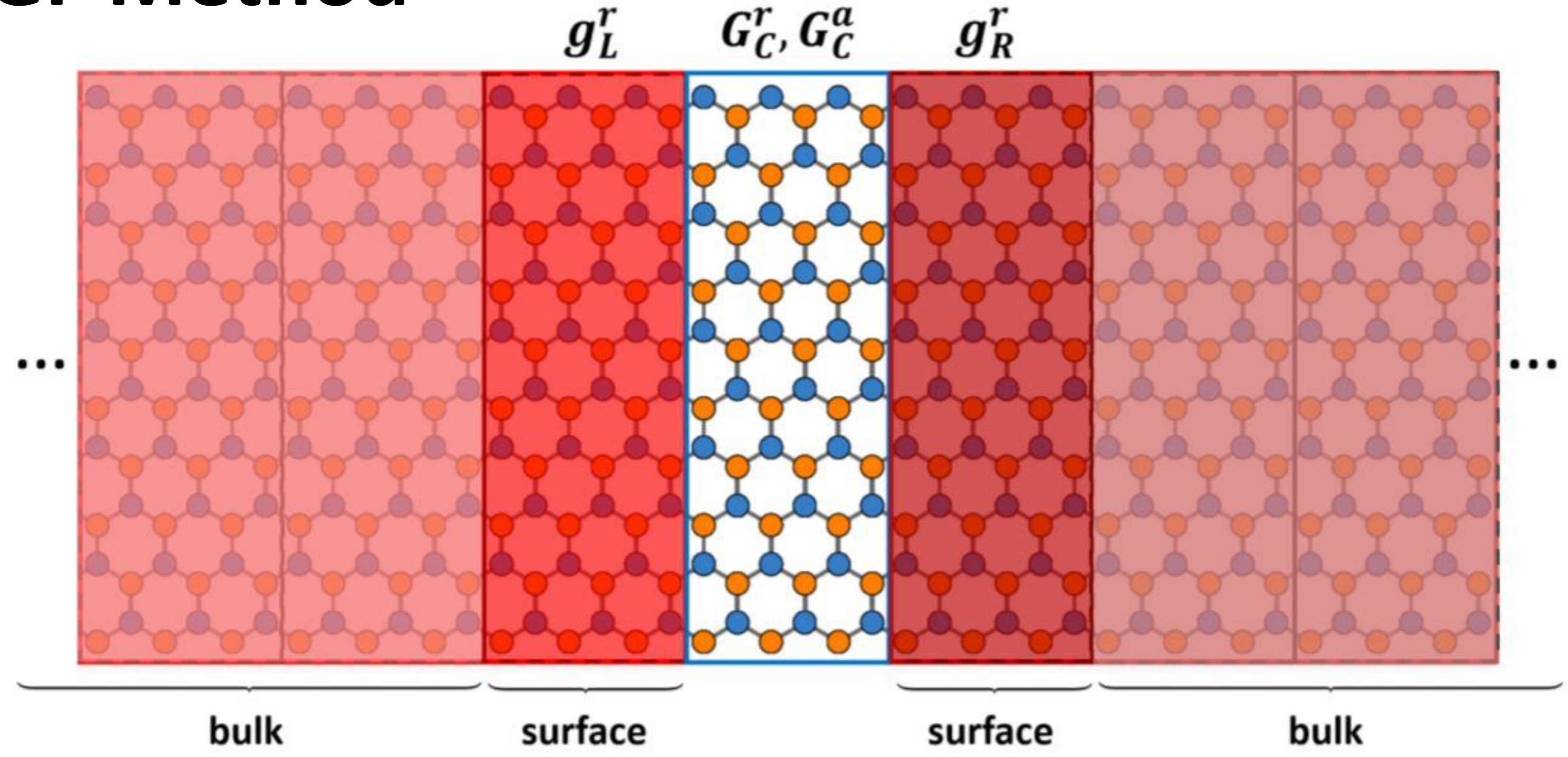
$$\Gamma(\omega)_\alpha = i(\Sigma_\alpha^r(\omega) - [\Sigma_\alpha^r(\omega)]^\dagger) \qquad \alpha = L,\ R$$



The NEGF Method



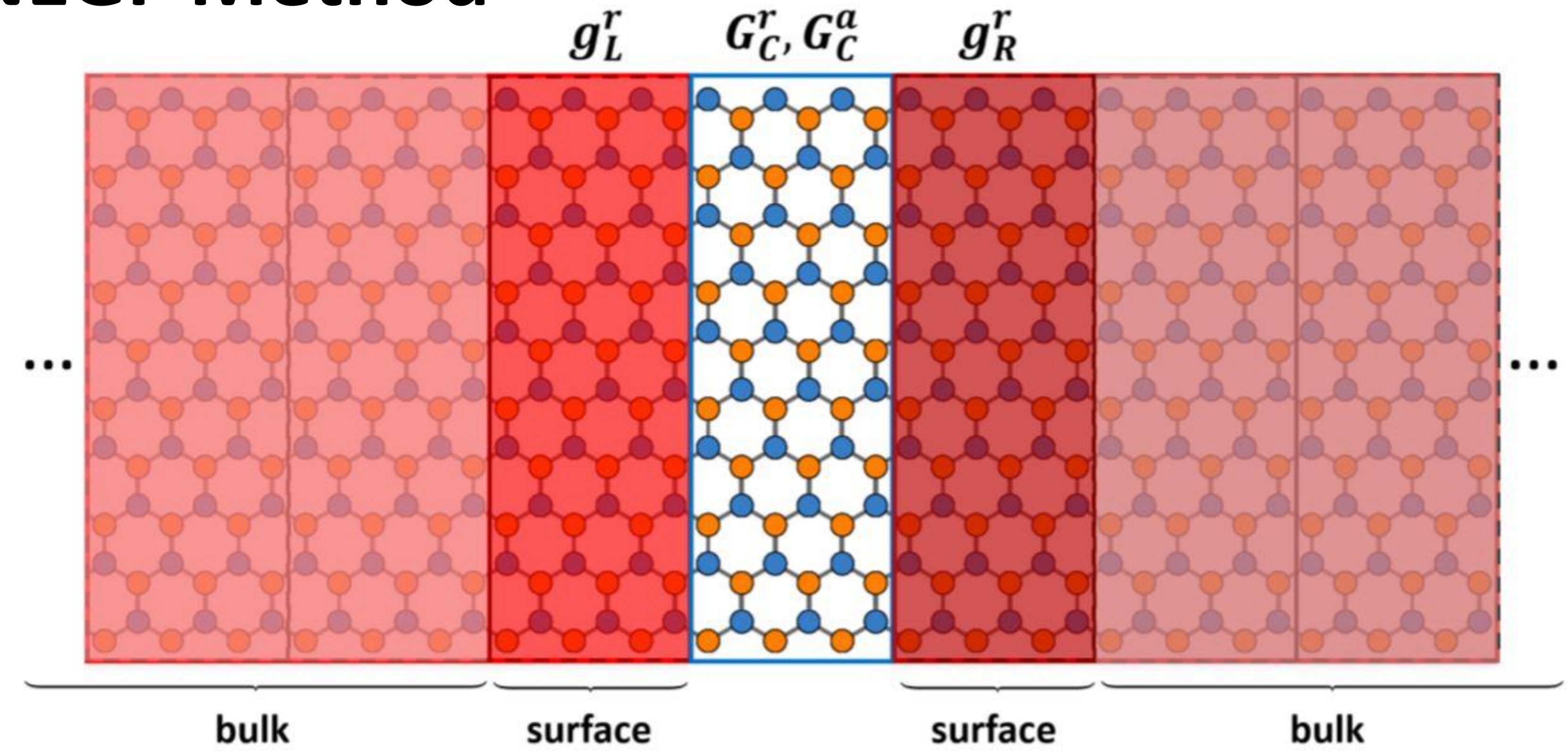
The NEGF Method



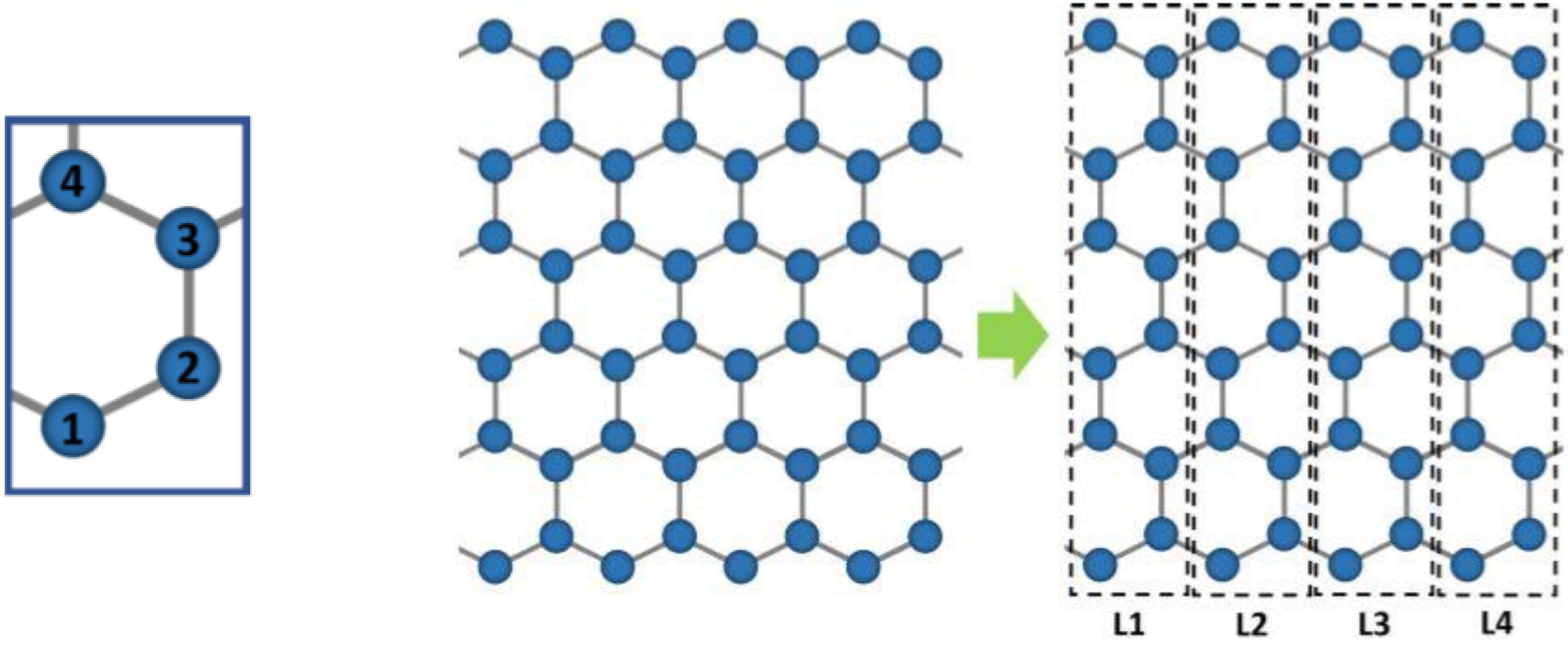
$$G_C^r = G^{CC} = \left[(\omega + i\eta_0\omega)^2 - K^C - \Sigma_L^r(\omega) - \Sigma_R^r(\omega)\right]^{-1}$$

$$\Sigma_\alpha^r = V^{C\alpha} g_\alpha^r(\omega) V^{\alpha C} \qquad \alpha = L,\ R$$

The NEGF Method



$$G^{\alpha C} = \underbrace{\left(\omega + i\eta\right)^2 - K^{\alpha}\Big]^{-1}}_{g_\alpha^r} V^{\alpha C} G^{CC}$$


4
3
2
1
L1
L2
L3
L4

Parameters used

Bond stretching force constants considered (in eV/($\mathring{A}^2$ amu))

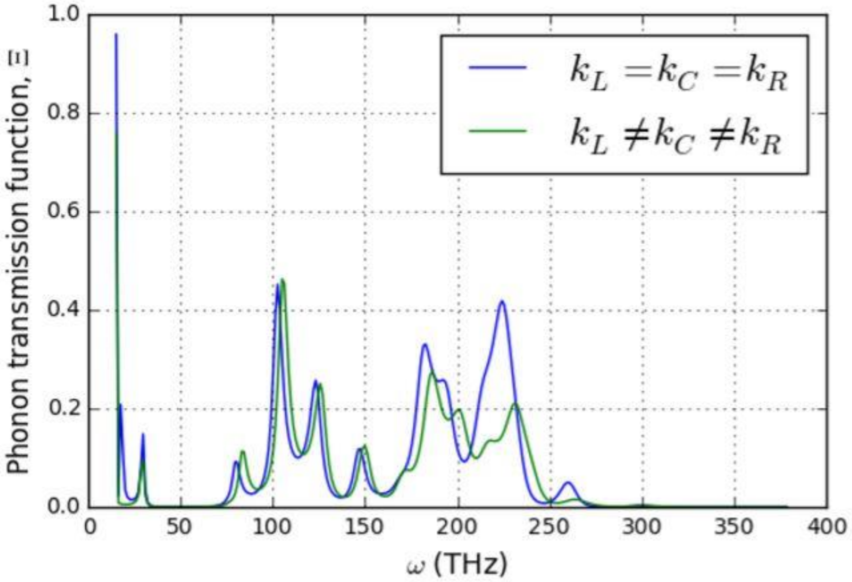
case	k_L	k_C	k_R
1	1.38	1.38	1.38
2	1.56	1.38	1.44

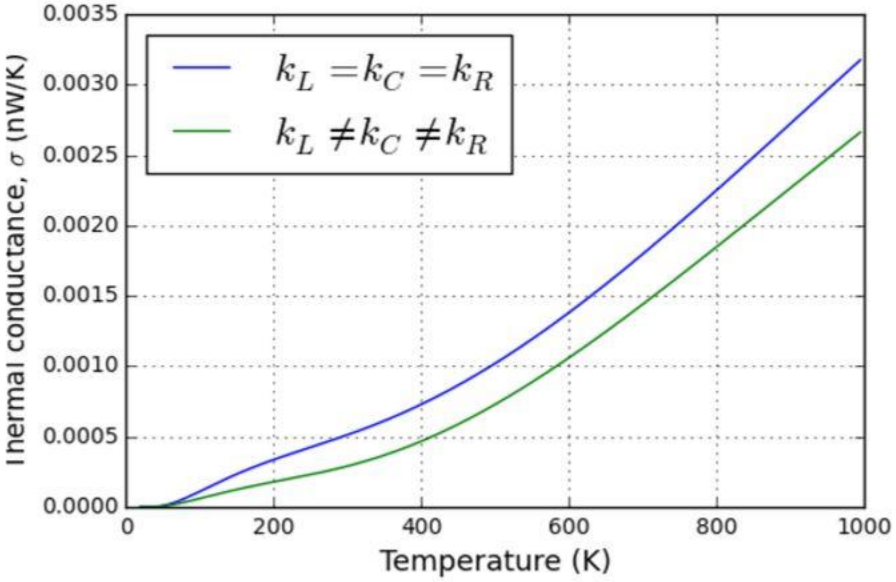
Force constants from carbon nanotube junctions:
J.-S. Wang, J. Wang & N. Zeng, *Phys Rev B* 74 (2006) 033408

	E (meV)	ω (THz)
minimum	10	15.2
maximum	250	380

Results

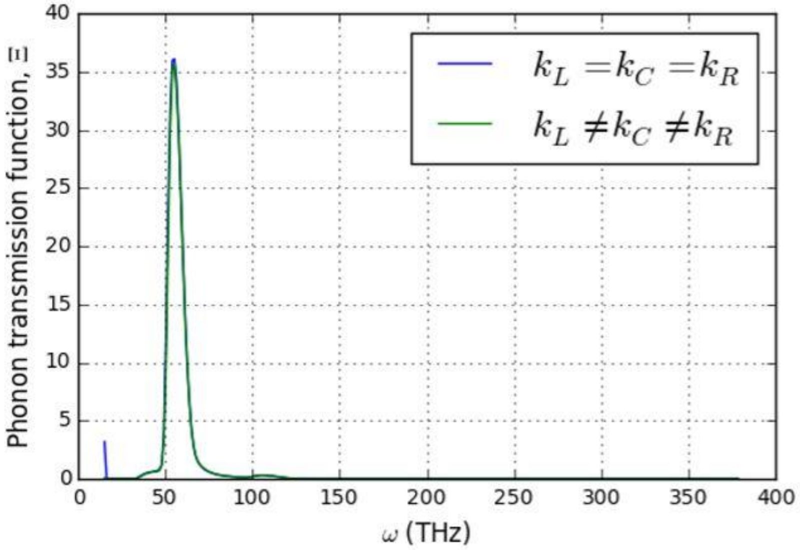
$l_0 \times \; w_0$

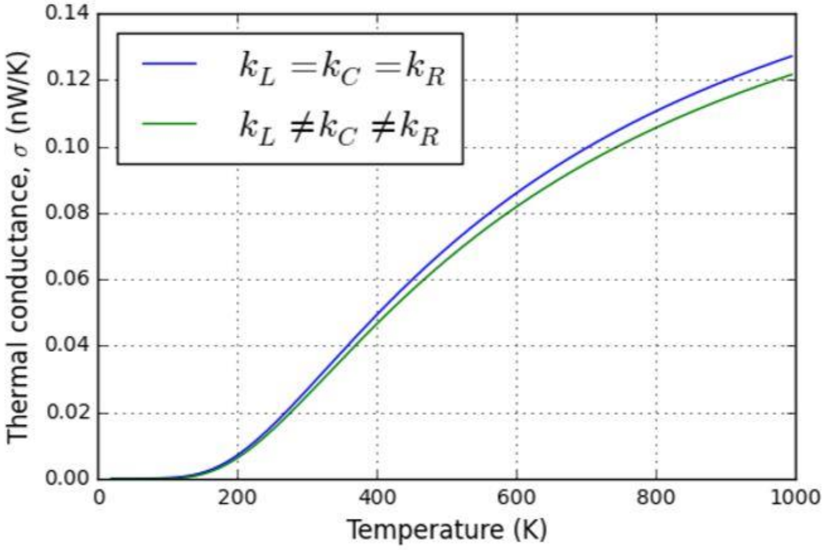




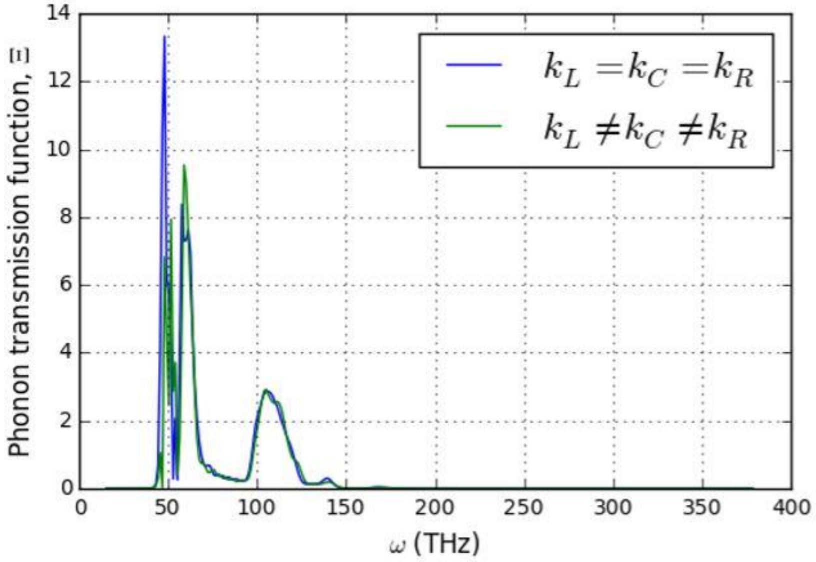
Results

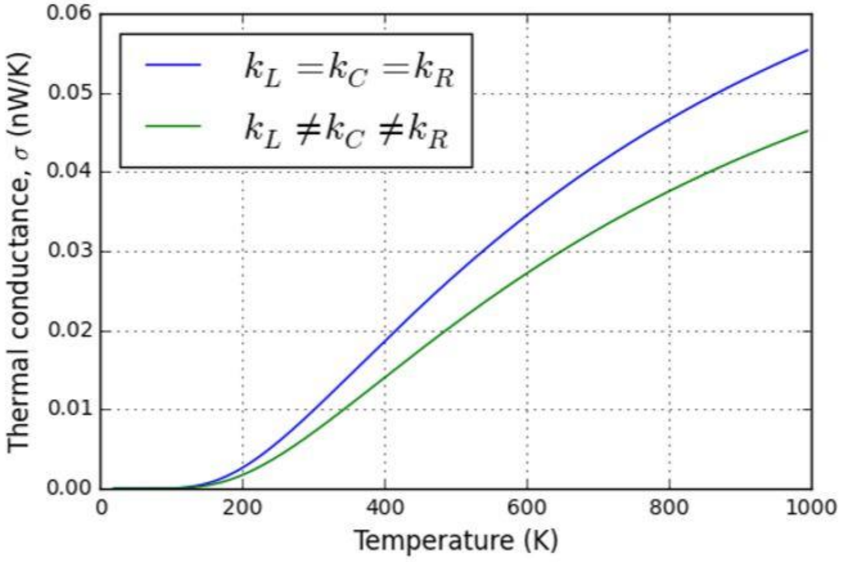
$16l_0 \times \ 8w_0$



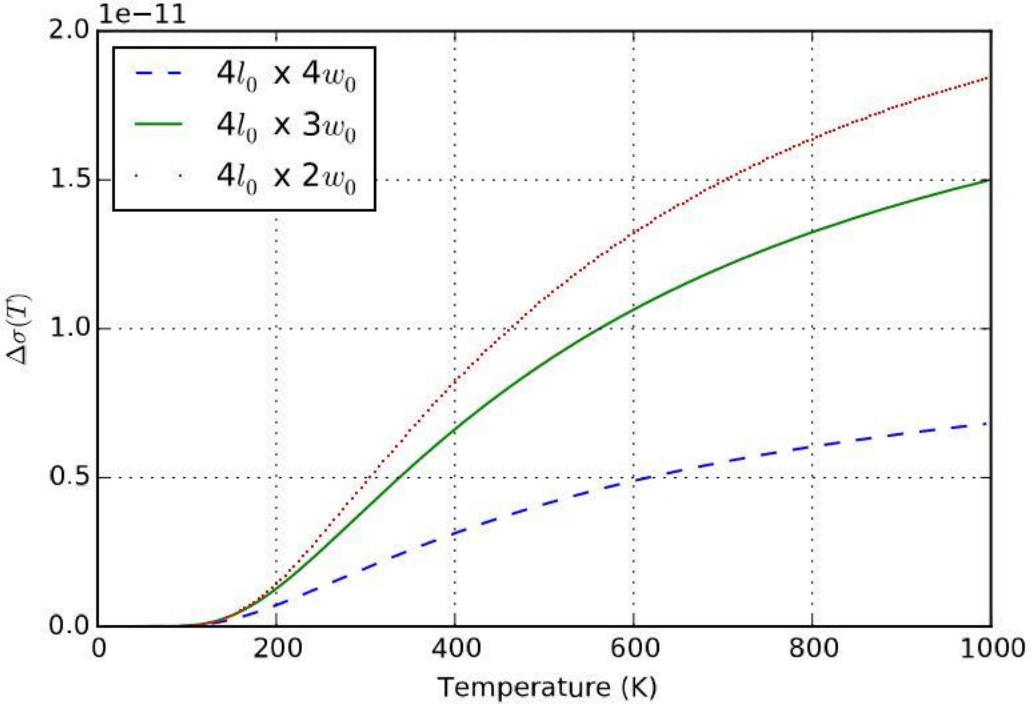


$5l_0 \times \ 2w_0$

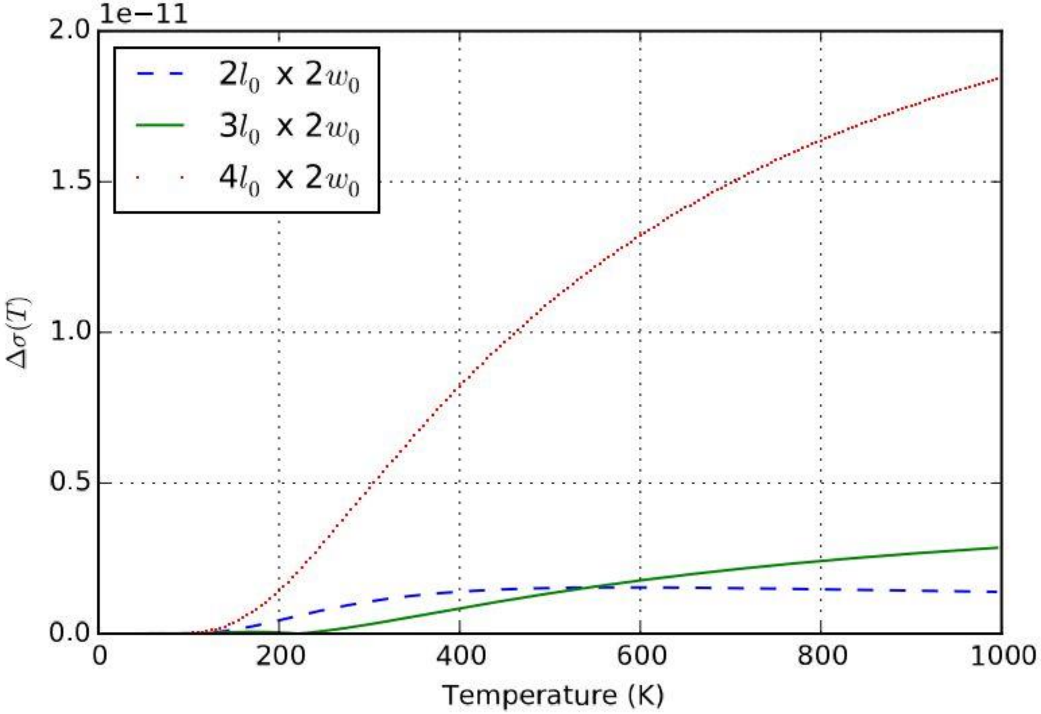




Results



1e−11
2.0
1.5
1.0
0.5
0.0
$\Delta\sigma(T)$
$4l_0$ x $4w_0$
$4l_0$ x $3w_0$
$4l_0$ x $2w_0$
0
200
400
600
800
1000
Temperature (K)

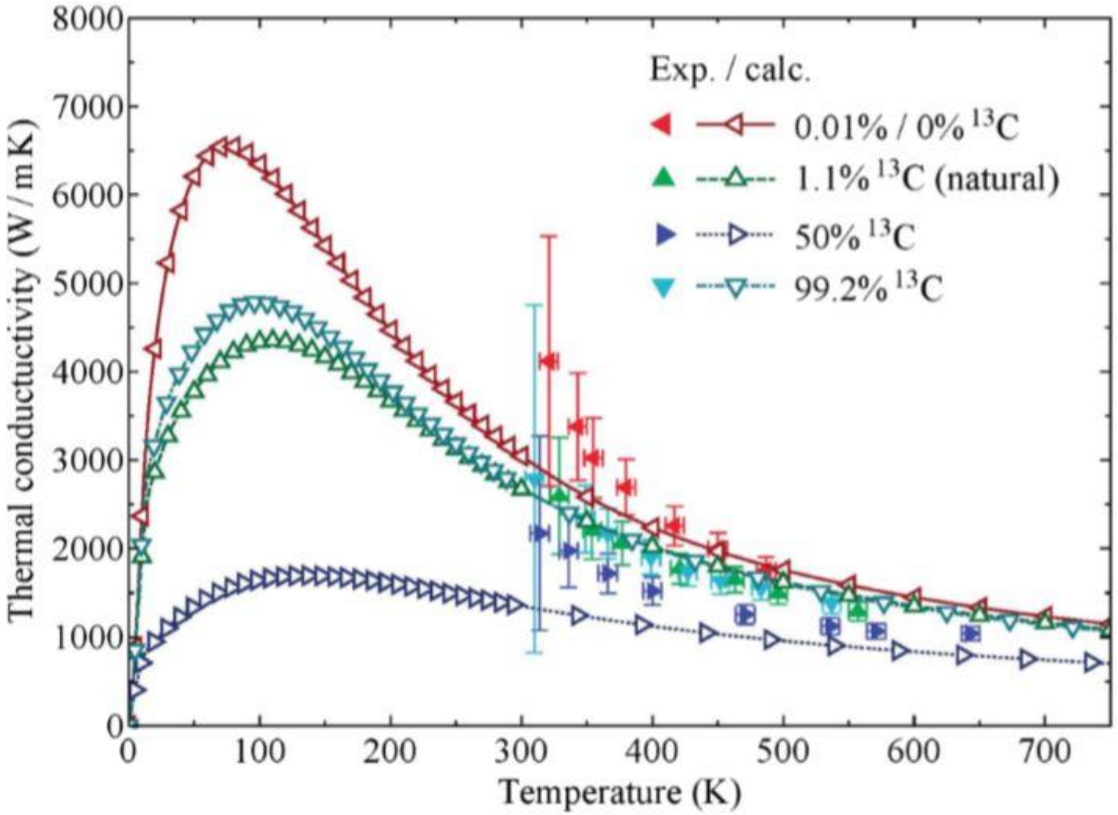


1e−11
2.0
1.5
1.0
0.5
0.0
$\Delta\sigma(T)$
$2l_0$ x $2w_0$
$3l_0$ x $2w_0$
$4l_0$ x $2w_0$
0
200
400
600
800
1000
Temperature (K)

What's next?

- accounting for 1.1% ^{13}C

$$\omega = \sqrt{\frac{\bar{m}_{\text{nat}}}{\bar{m}}}\omega_{\text{nat}}.$$



R. Saito, M. Mizuno & M.S. Dresselhaus, *Phys. Rev. Applied* 9 (2018) 024017

Thank you.

SanD

The Structure and Dynamics Group

http://www.nip.upd.edu.ph/sand