MULTISCALE THERMAL MODELS OF NANOSTRUCTURED DEVICES

Giuseppe Romano

PhD dissertation

XXII CICLO

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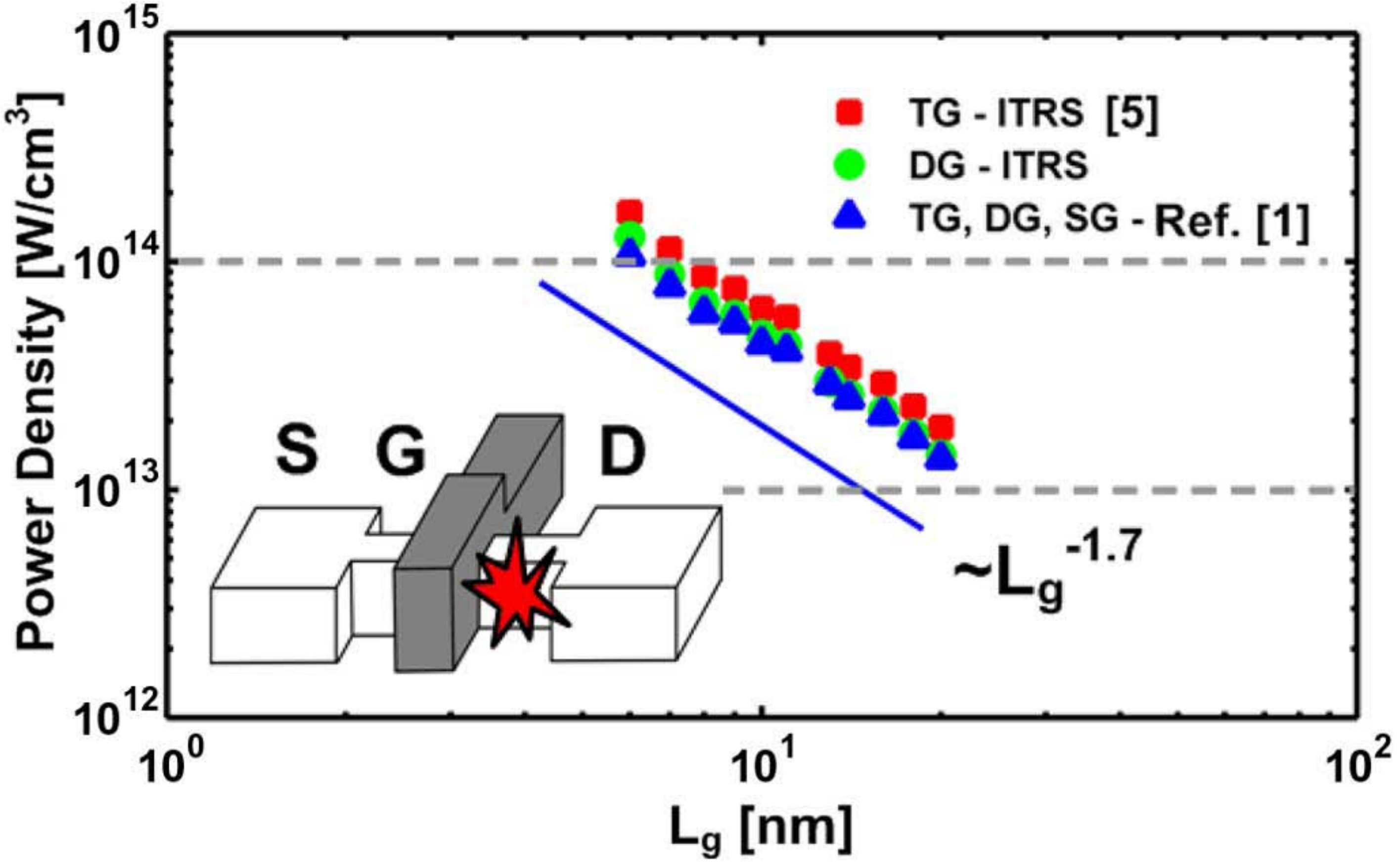
COORDINATOR:
Prof. Giuseppe Bianchi

OLABs

03/06/2010

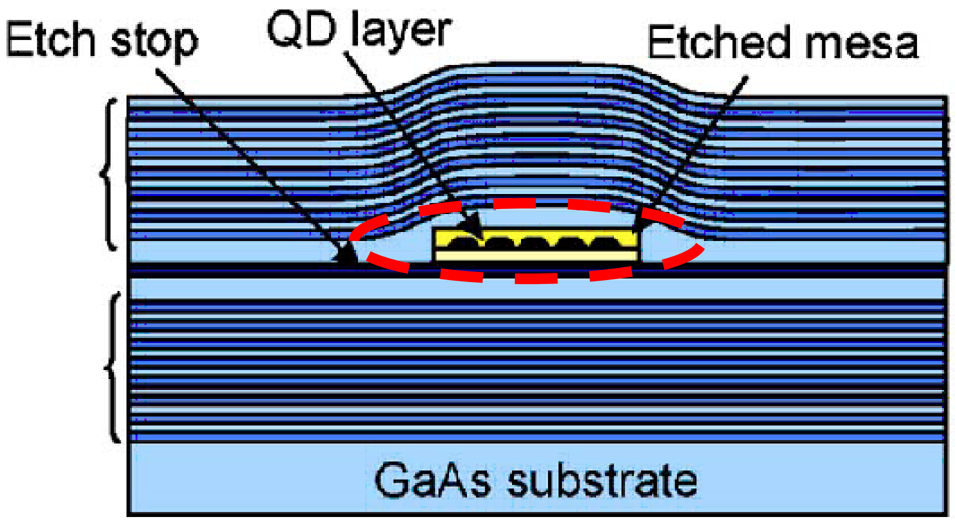
UNIVERSITA' DEGLI STUDI DI ROMA Tor Vergata

INTRODUCTION



Goodson et al. IEEE Elect. Lett. (2008)

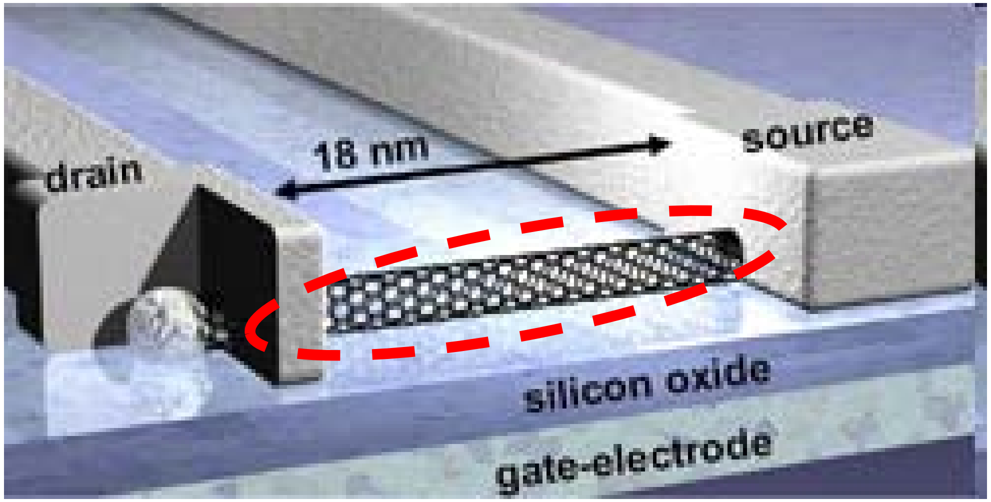
INTRODUCTION



Quantum DOTs based MESA

Muller et al. APL (2006)

Carbon nanotube based transistor



Infineon

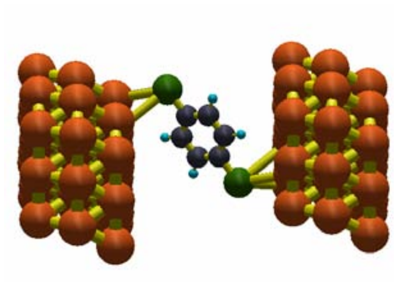
OUTLINE

- Introduction
- Heat transfer at the nano scale
- Heat transfer at the meso scale
- Heat transfer at the macro scale
- Multiscale model
- Conclusion

Scales

Phonon wavelength

$\lambda \approx 10nm$



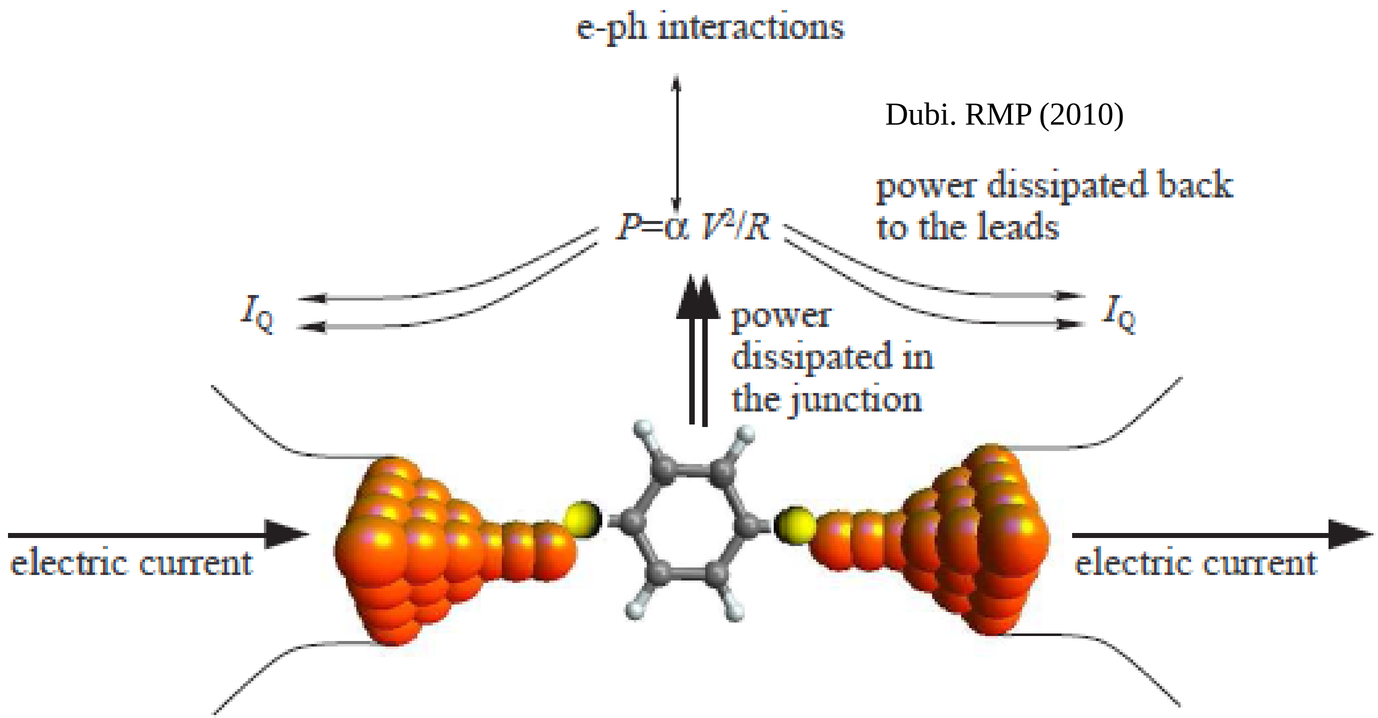
Nanoscale

L

P_D ?

P_E ?

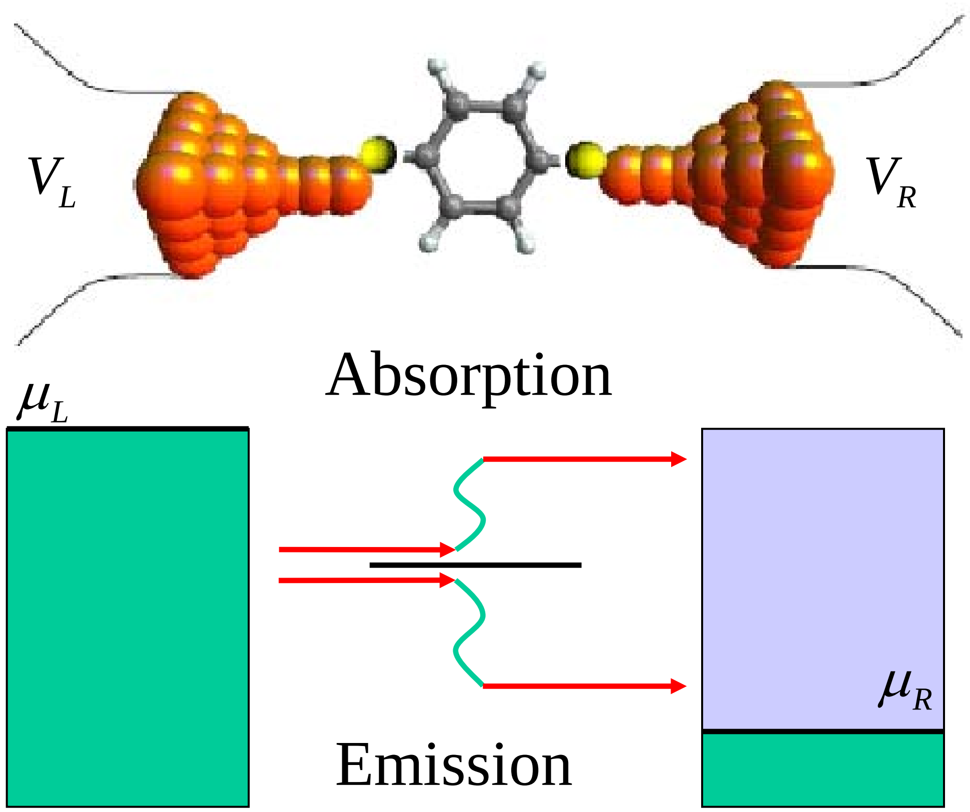
Heat balance at the nanoscale



The internal energy is stored and dissipated by phonons

The vibration is splitted in 3N-6 normal modes (q-labeled).

Heating at the nanoscale



[A. Pecchia et al. Report on Progress in Physics (2004)]

Cross sections

Phonon-phonon interaction

[G. Romano, A. Pecchia and A. Di Carlo **J. of Physics: cond. matt.** (2007)]

$$P_D^q = \hbar\omega_q \sum_{\alpha} \Lambda_q^{\alpha} (N_q - n_q^{\alpha})$$

$$P_E^q = \hbar\omega_q \left[E_q (N_q + 1) - A_q N_q \right]$$

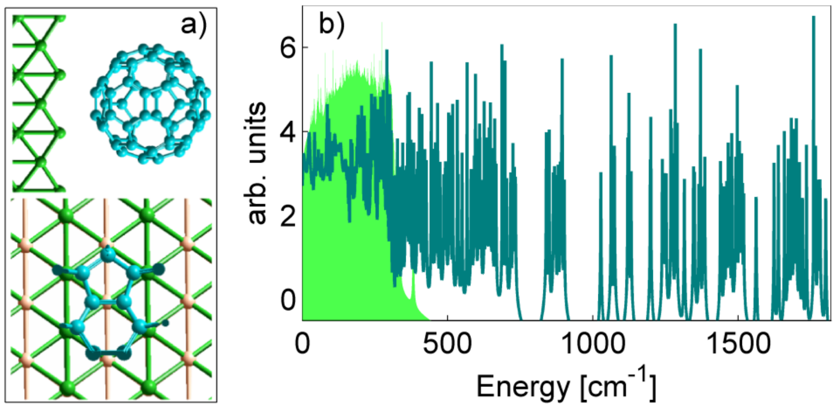
$\Rightarrow N_q \Rightarrow T_{mol}$

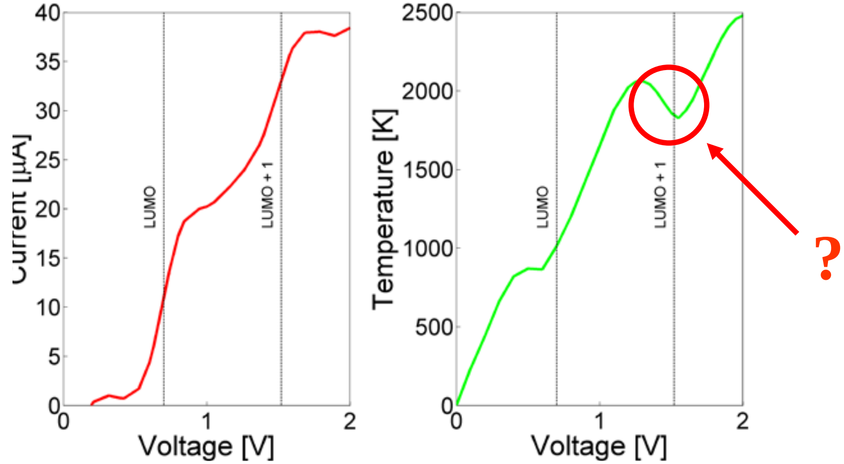
Electron-phonon interaction

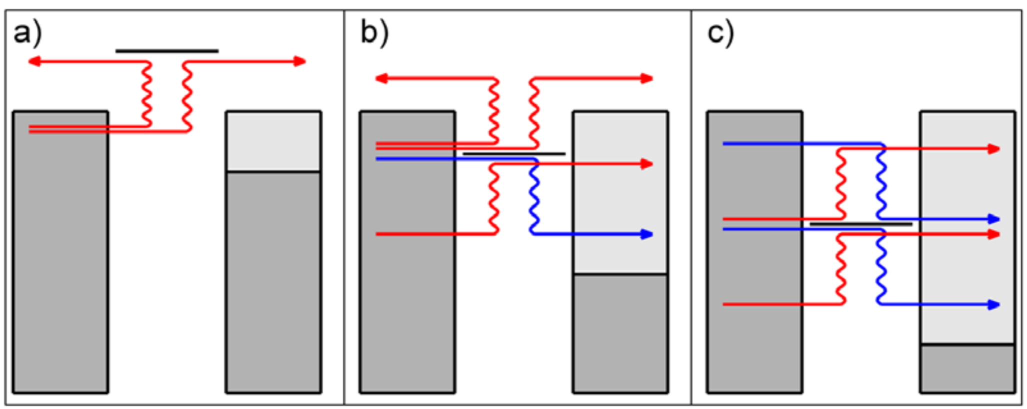
[A. Pecchia, G. Romano and Aldo Di Carlo **Physical Review B** (2007)]

Transport model	⇒	Non equilibrium Green's Function (NEGF)
Ground state	⇒	Density Functional Theory (DFT)
Electron-phonon interaction	⇒	Born Approximation (BA)

Resonance effect





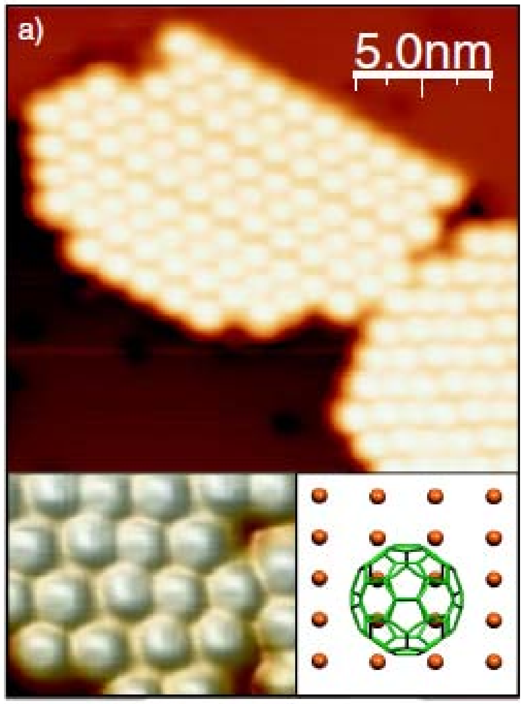


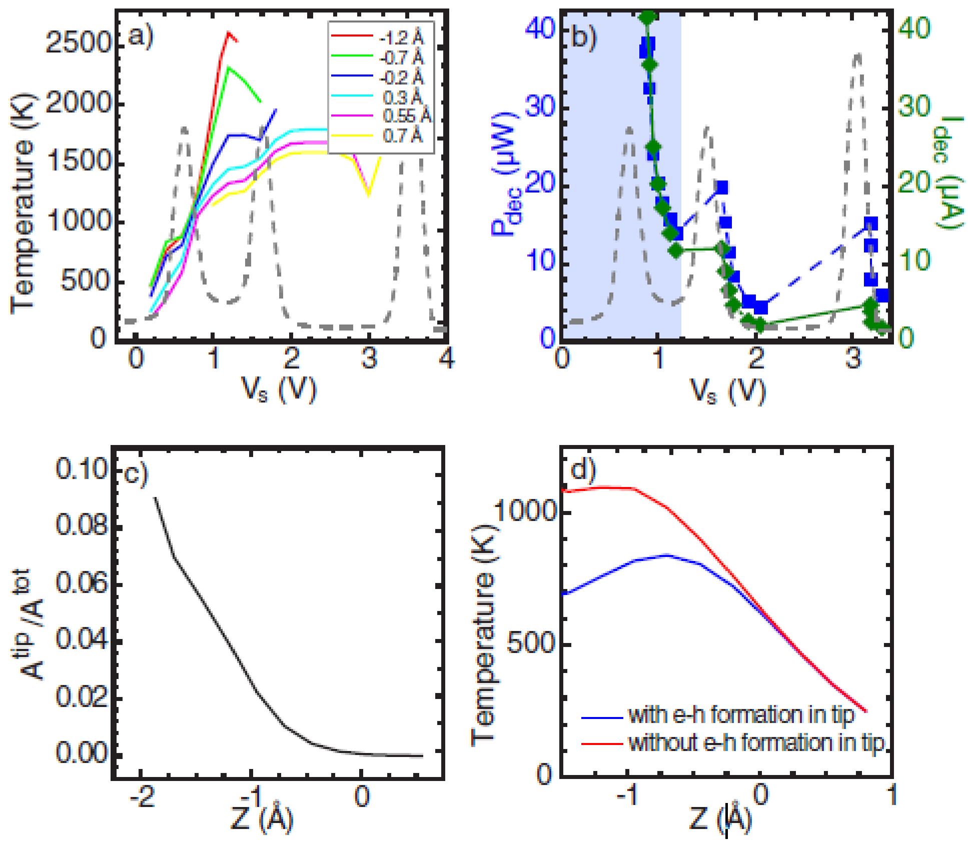
The absorption can prevail over the emission and cools the molecule

[G. Romano, A. Gagliardi, A. Pecchia and Aldo Di Carlo et al. **Physical Review B** (2010)]

Collaboration with experimentalists

Thermal instability of fullerenes



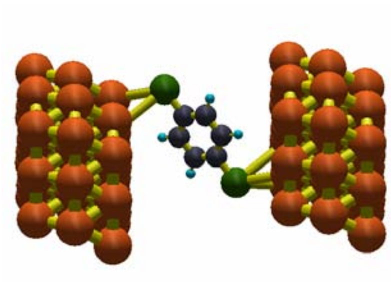


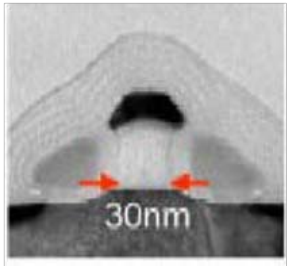
[G. Schulze, K. Franke, A. Gagliardi, G. Romano, C. Lin, A. Rosa, T. A. Niehaus, T. Frauenheim, A. Di Carlo, A. Pecchia and J. Pascual. **Physical Review Letters** (2009)]

Scales

Phonon wavelength
$\lambda \approx 10nm$

Phonon mean free path
$\Lambda \approx 100nm$





	Nanoscale	Mesoscale
P_D	$\sum_q \sum_\alpha \Lambda_q^\alpha (N_q - n_q^\alpha)$	?
P_E	$\sum_q E_q (N_q + 1) - A_q N_q$	?

L

Heat balance at the mesoscale: the gray model

$$v_g \nabla\left(\vec{s} e''\right) = \frac{e^0 - e''}{\tau} + \tilde{H}$$

Equilibrium energy $\Rightarrow$ $e^0 = \frac{1}{4\pi}\int_{4\pi} e'' d\Omega$

Thermal flux $\Rightarrow$ $\vec{J} = \int_{4\pi} \vec{s} v_g e'' d\Omega$

Temperature $\Rightarrow$ $T = T_0 + \frac{4\pi e^0}{C}$

- All phonons are assumed to have the same group velocity (sound velocity)
- Relaxation time is indipendent of energy phonons.
- Discontinuous Galerkin Method

[Sreekant et al. Heat and Mass Transfer (2006)]

Equilibrium energy

•Since the equilibrium energy depends on the solution itself a self consistent loop is required.

•The first guess of the equilibium energy is a key point for the convergence speed.

Usual choice:

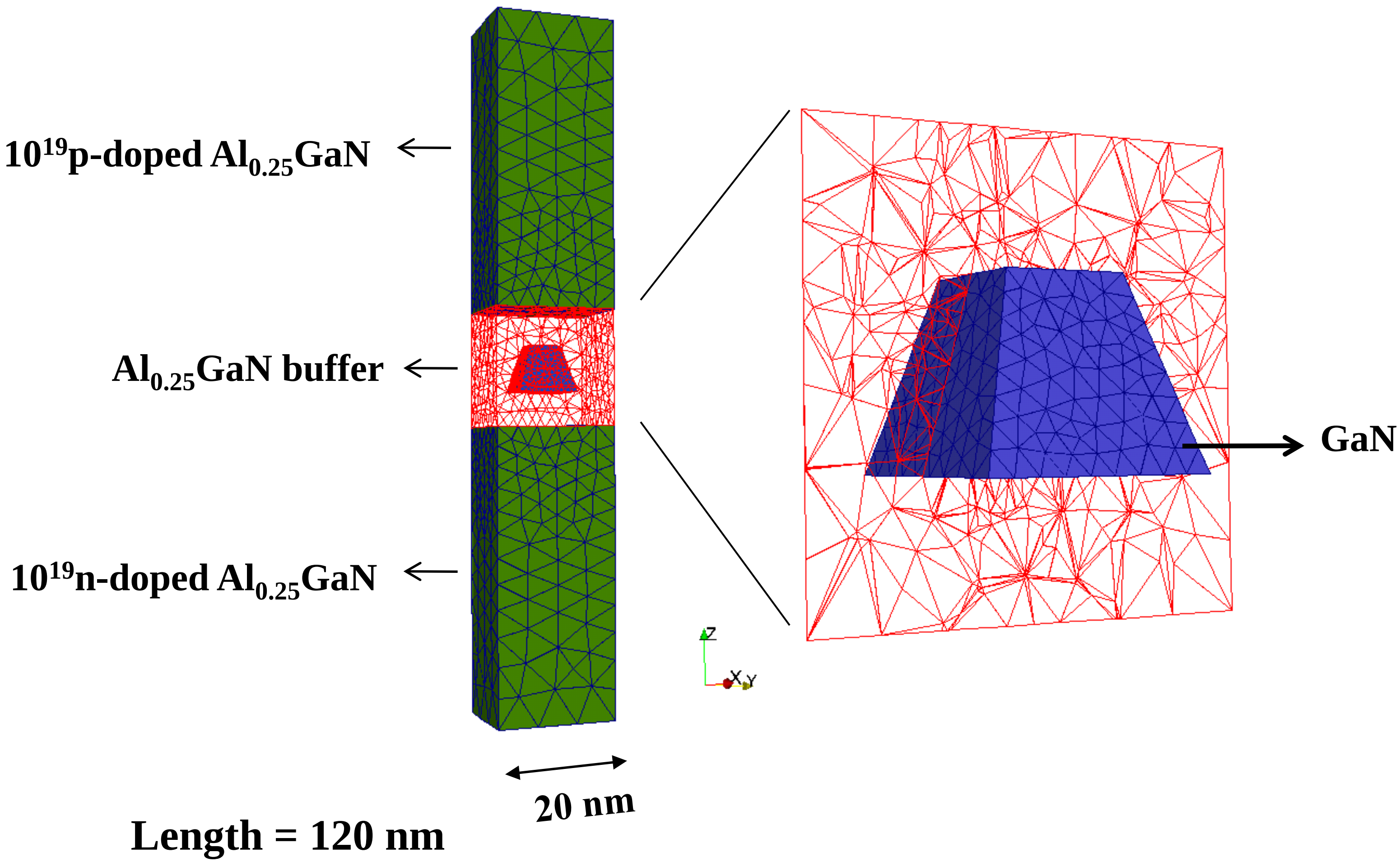
constant value ⇒ 1000 steps

This work:

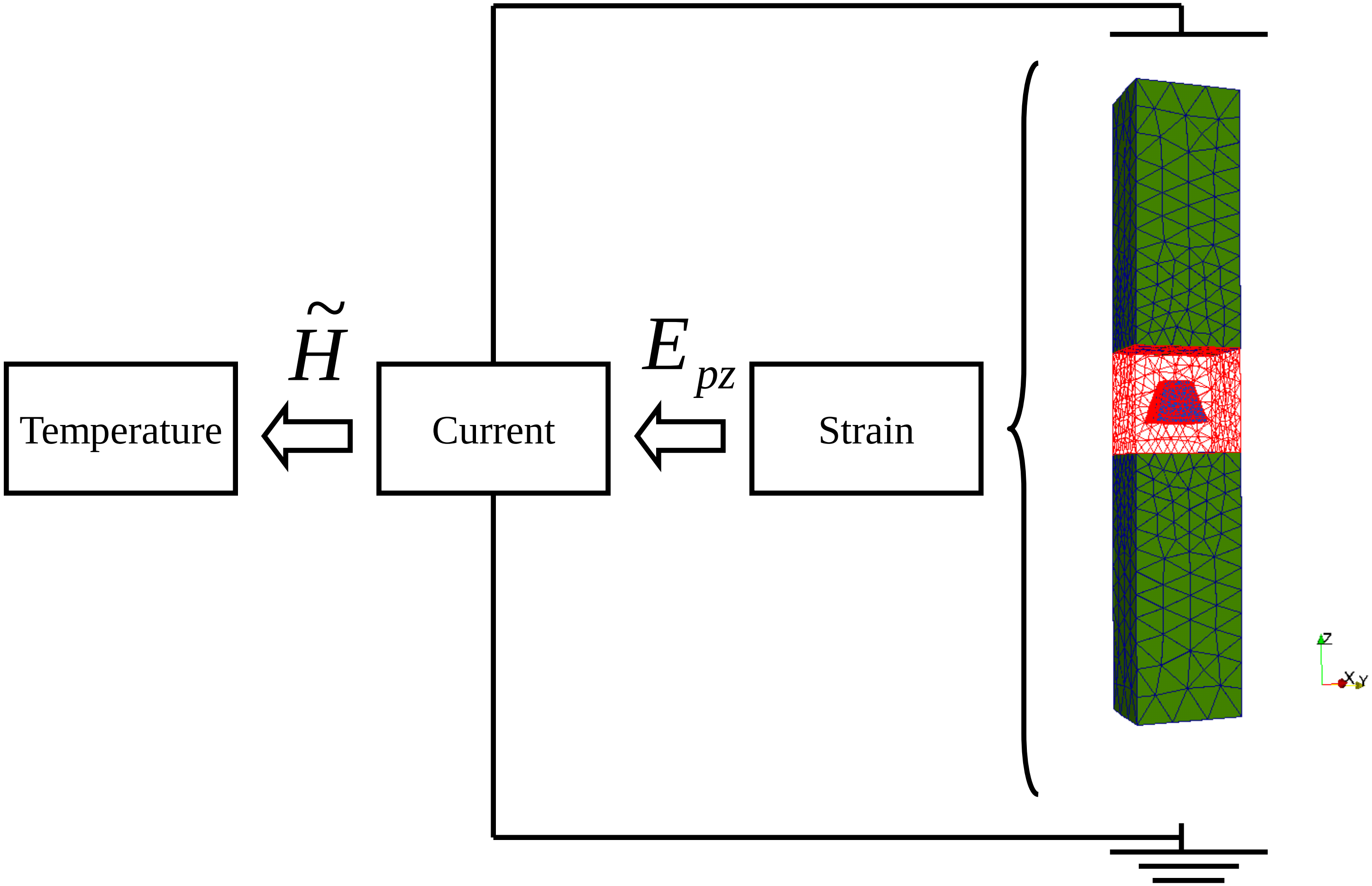
Fourier simulation ⇒ 10 steps

This approach speeds the convergence up to 100 times

GaN quantum dot

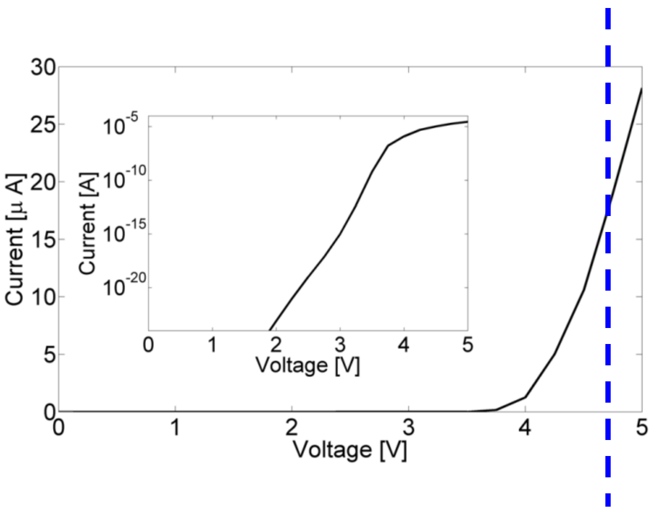


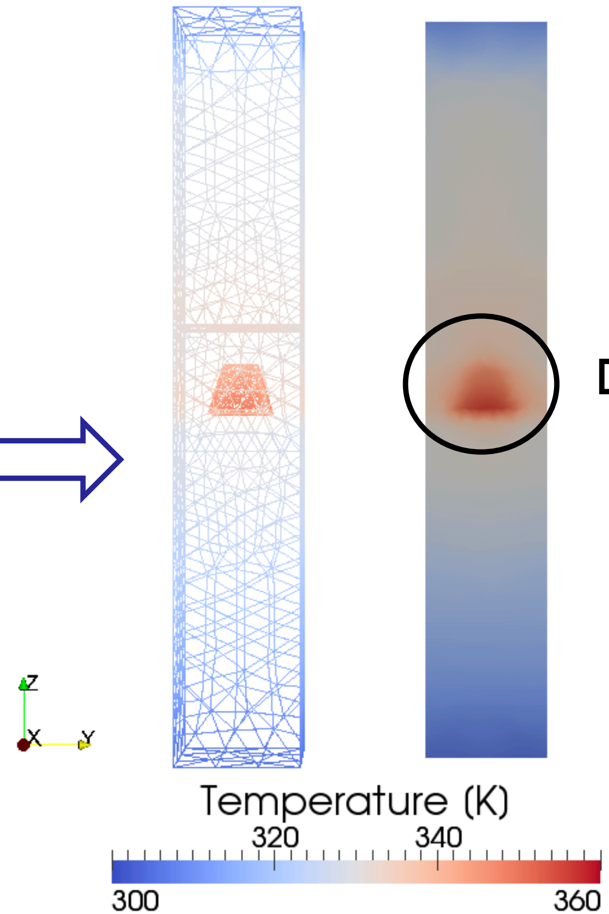
GaN quantum dot: meso results



GaN quantum dot: meso results

The solid angle is discretized in 18 slices

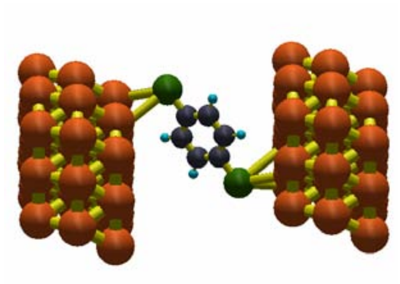


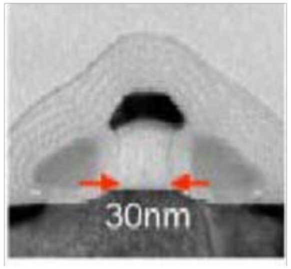


$$T_M^B \approx 358K$$

Scales

Phonon wavelenght $\lambda \approx 10nm$ | Phonon mean free path $\Lambda \approx 100nm$





	Nanoscale	Mesoscale	Macroscale
P_D	$\sum_q \sum_\alpha \Lambda_q^\alpha (N_q - n_q^\alpha)$	$\int_{4\pi} \nabla \cdot \left(v_g e''\mathbf{s}\right) d\Omega$	?
P_E	$\sum_q E_q (N_q + 1) - A_q N_q$	$\int_{4\pi} \tilde{H}(\Omega) d\Omega$	?

L

Thermal transport at the macroscales

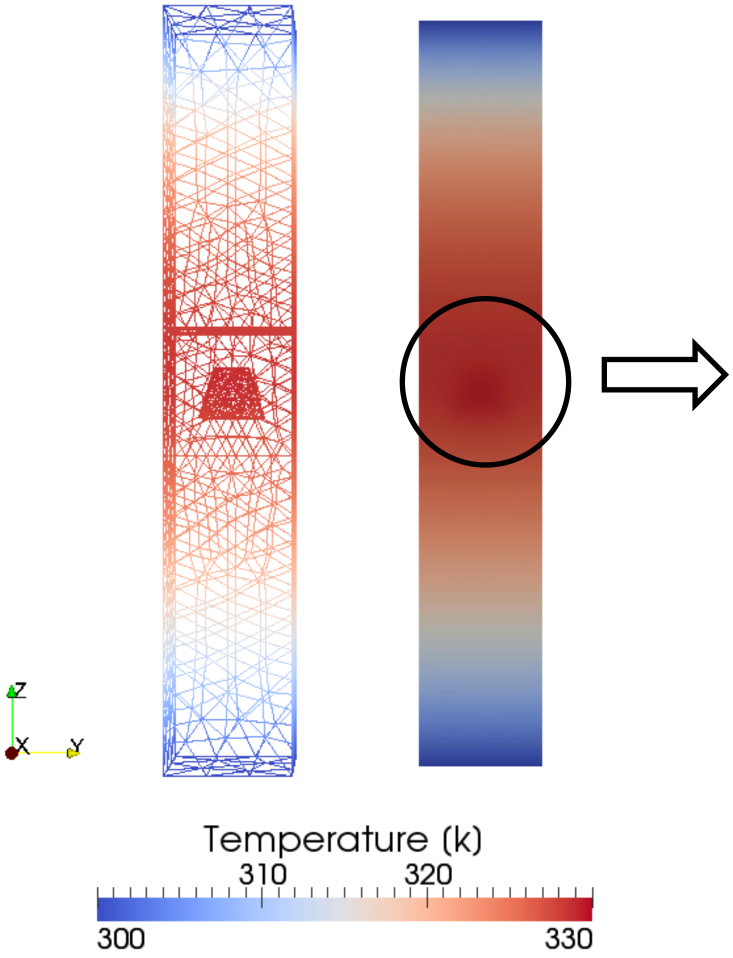
Irreversible thermodynamics
Onsager reciprocity relationships
Local thermal equilibrium
Standard Galerkin Method

$$\nabla \cdot \left(\kappa \nabla T \right) = H$$

$$H_n = \frac{\left| J_n \right|^2}{\sigma_n}$$

$$H_p = \frac{\left| J_p \right|^2}{\sigma_p}$$

$$H_{rec} = e\left(\phi_n - \phi_p \right) R$$

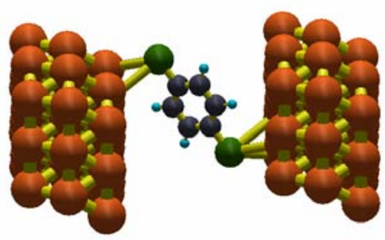


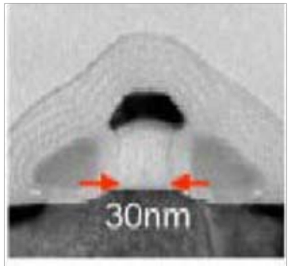
$$T_M^F \approx 319K$$

Scales

Phonon wavelenght
$\lambda \approx 10nm$

Phonon mean free path
$\Lambda \approx 100nm$

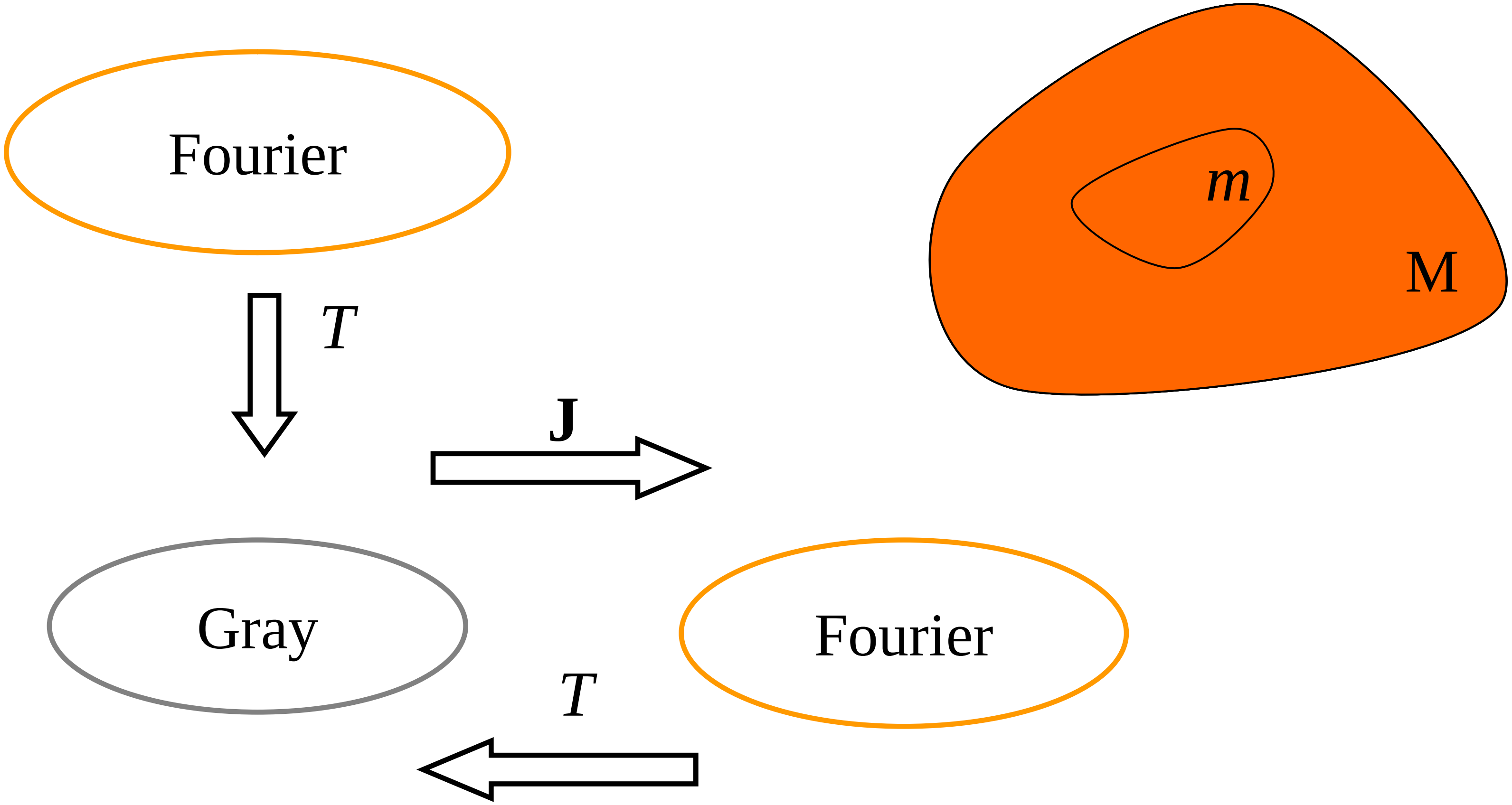




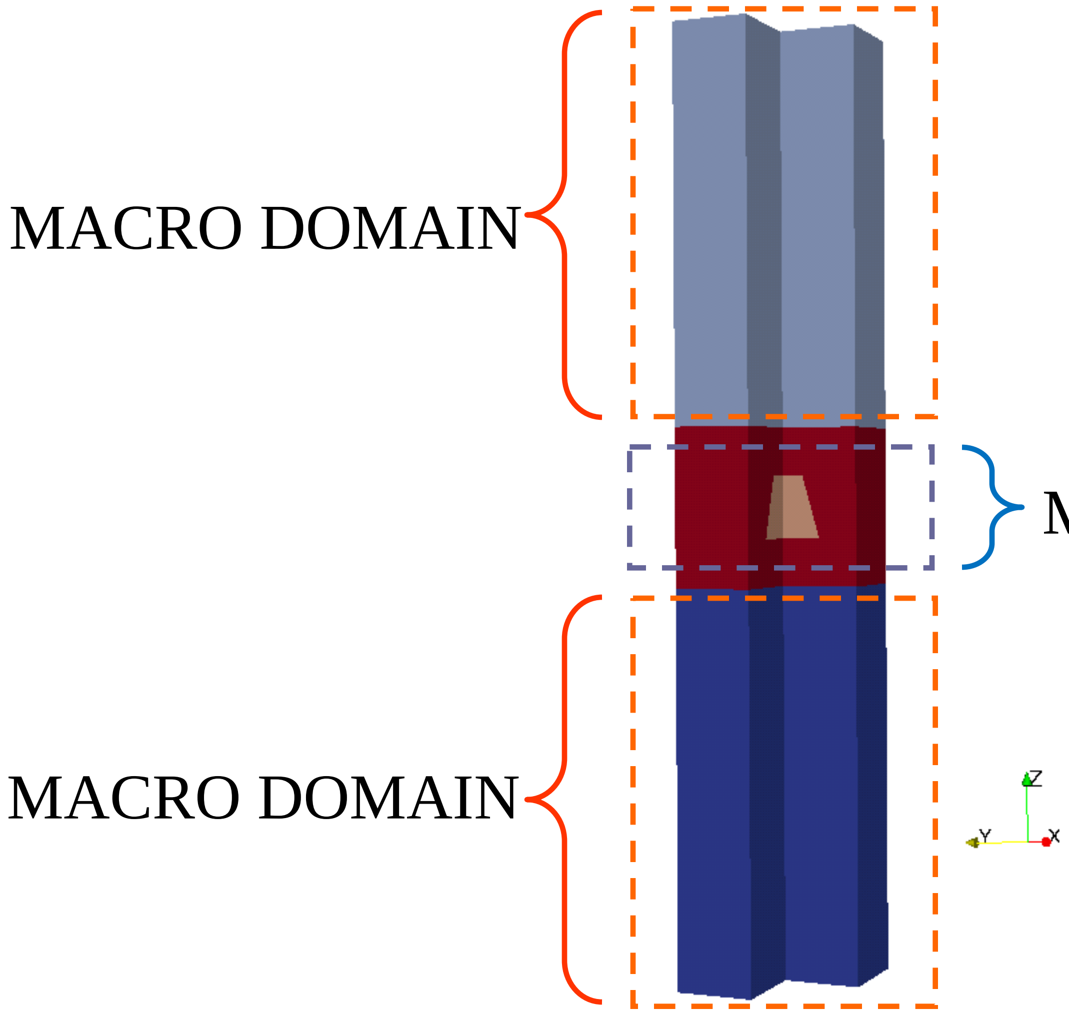
	Nanoscale	Mesoscale	Macroscale
P_D	$\sum_q \sum_\alpha \Lambda_q^\alpha (N_q - n_q^\alpha)$	$\int_{4\pi} \nabla \cdot \left(v_g e''\mathbf{s}\right) d\Omega$	$\nabla \cdot \left(\kappa \nabla T\right)$
P_E	$\sum_q E_q (N_q + 1) - A_q N_q$	$\int_{4\pi} \widetilde{H}(\Omega) d\Omega$	H

L

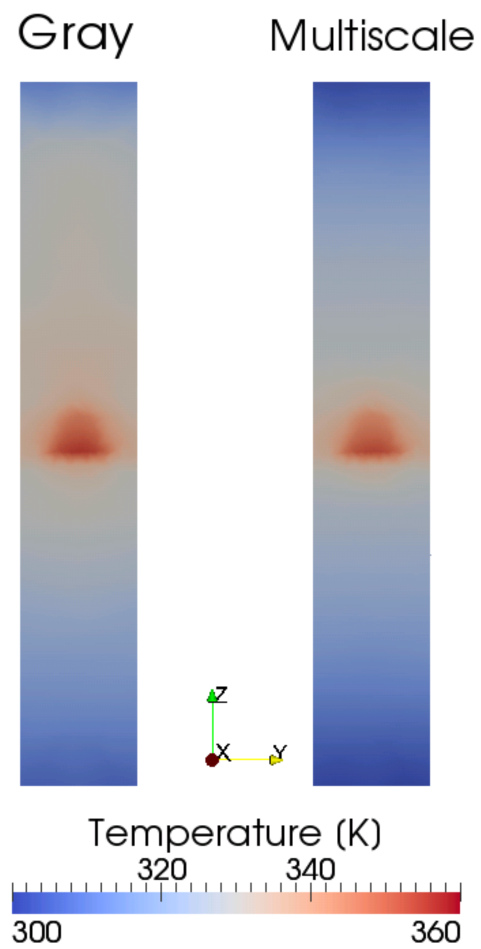
THE METHOD

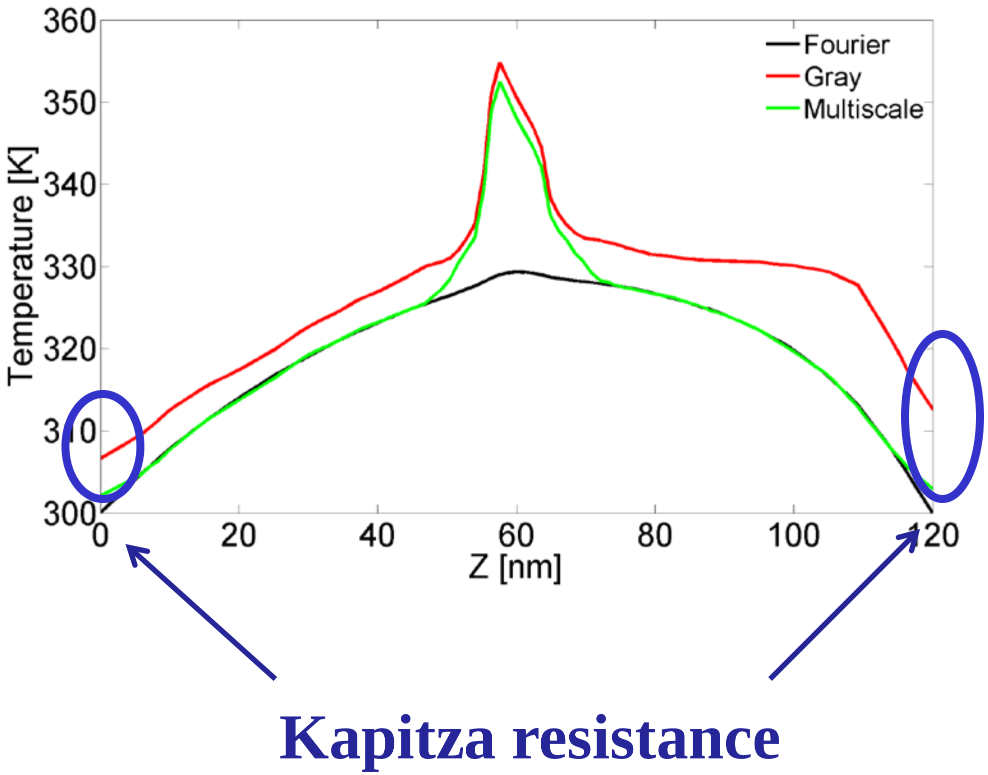


Domain partitioning



Multiscale model: results

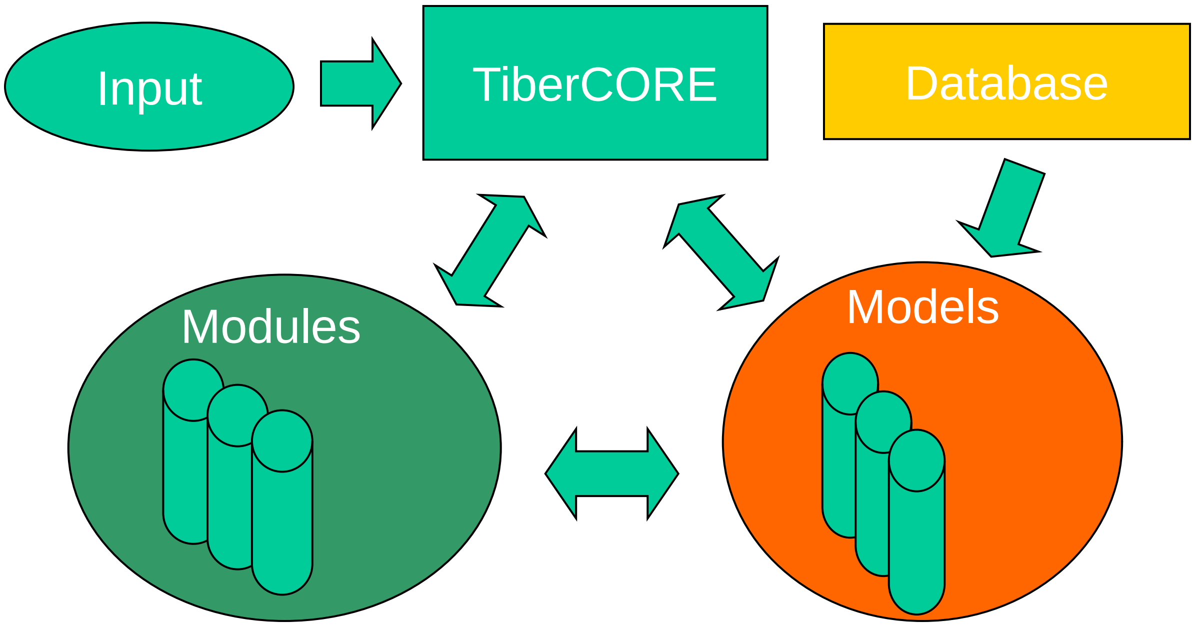




G. Romano, A. Pecchia and A. Di Carlo**. IEEE Journal of Quantum Electronics** (in preparation)

TiberCAD

The models have been implemented in TiberCAD, a multiscale simulator of optoelectronic devices.



www.tibercad.org

Conclusion

Developed and implemented a model for heating and heat dissipation at the nanoscale (NEGF-DFT)

Implemented and optimized a Boltzmann based model for electro-model simulation (Discontinuous Galerkin Method)

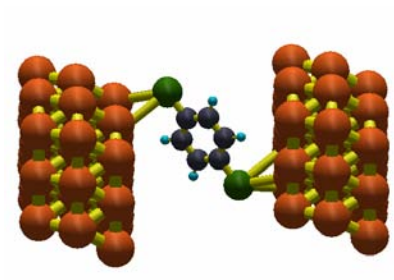
Implemented the Fourier’s law for heat transport (Standard Galerkin Method)

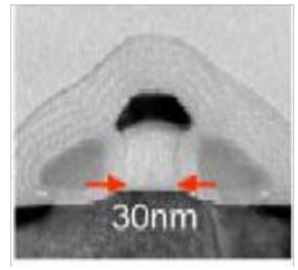
Developed and implemented the Macro/Meso multiscale model.

Application of the implemented models to several systems, ranging from molecular structures to macro devices.

Future work

Phonon wavelenght	Phonon mean free path
$\lambda \approx 10nm$	$\Lambda \approx 100nm$

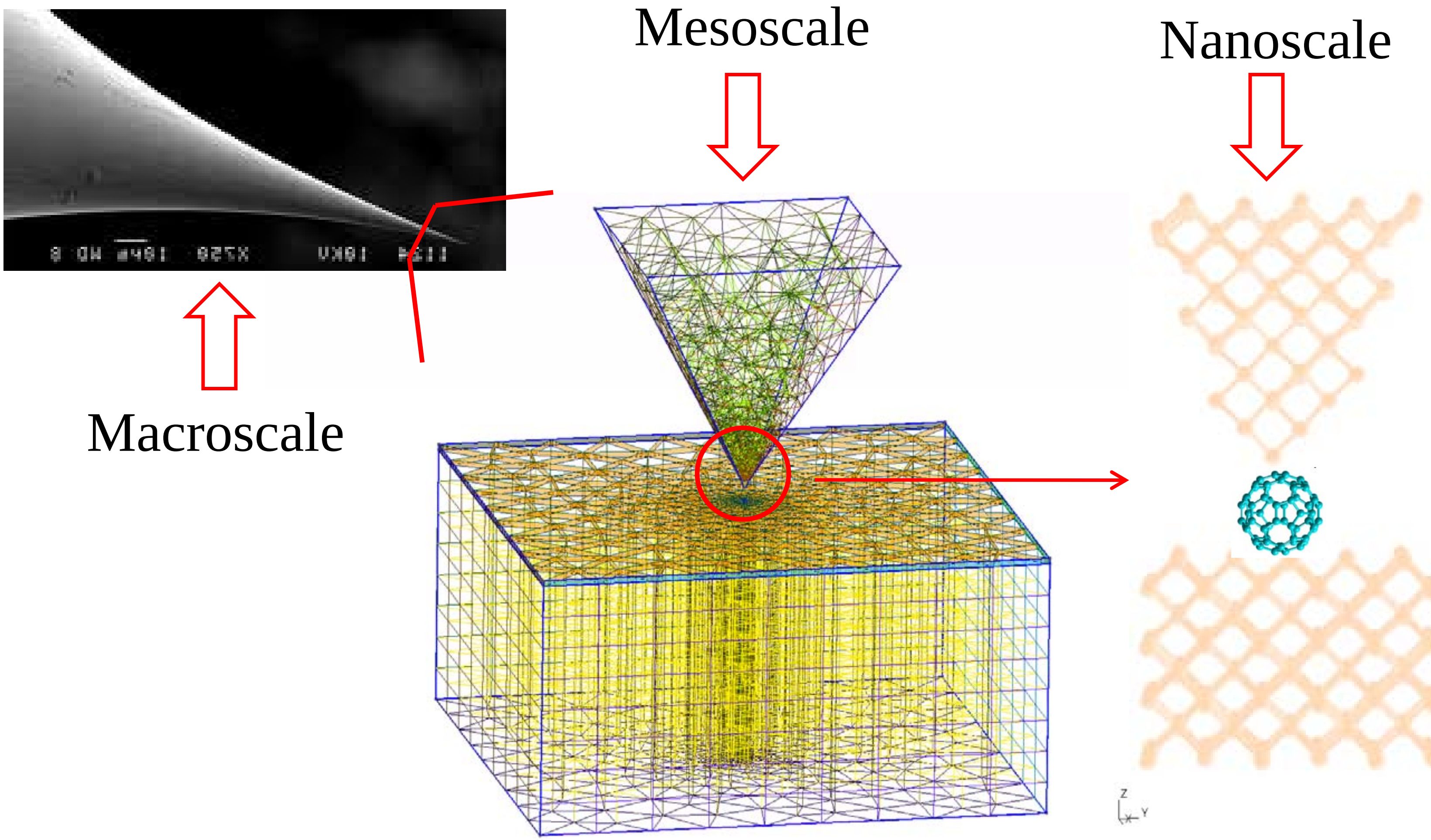




	Nanoscale	Mesoscale	Macroscale
P_D	$\sum_q \sum_\alpha \Lambda_q^\alpha (N_q - n_q^\alpha)$	$\int_{4\pi} \nabla \cdot (v_g e'' \mathbf{s}) d\Omega$	$\nabla \cdot (\kappa \nabla T)$
P_E	$\sum_q E_q (N_q + 1) - A_q 1$	$\int_{4\pi} \widetilde{H}(\Omega) d\Omega$	H

L

Full integration



Visiting scholarships

08/2009-10/2009

Georgia Institute of Technology, Atlanta, GA (USA)
Supervisor: Prof. Zhong Lin Wang
Activities:

- FEM simulation of piezoelectric nanogenerators and nanopiezotronic devices.
- Investigation on energy harvesting for nanoelectronics
- Collaboration with experimentalists.

08/2008-10/2008

Kyoto Institute of Technology, Kyoto (JAPAN).
Supervisor: Prof. Giuseppe Pezzotti
Activities:

- FEM simulation of Raman shift induced by the internal stress.
- Investigation on phonon deformation potentials.
- Collaboration with experimentalists.

DIDACTIC ACTIVITIES

GE2008: Nanophotonics and Nanoelectronics: technologies, devices and applications. 18-20 June, 2008. Otranto (Italy).

International Summer School on Advanced Microelectronics. MIGAS 2007. Grenoble (France), 2007.

Metodi e modelli per la matematica applicata. Prof. Vieri Mastropietro. June-july 2007.

Dispositivi Elettronici. Prof. Arnaldo D’amico, 2007.

Scuola di Dottorato. Nanoelectronic Modeling: electronic structure and transport at the nanoscale. Prof. Gerhard Klimeck. 5-9 October, 2009

PRESENTATIONS

G. Romano, G. Mantini, A. Di Carlo, A. D'Amico, C. Falconi and Z. L. Wang. *Simulation of piezoelectric nanogenerators with TiberCAD.* AISEM 2010, **Messina (Italy),** 8–10, Feb 2010 (Poster).

G. Romano, G. Penazzi and A. Di Carlo. *Multiscale thermal modeling of GaN/AlGaN quantum DOT LEDs*. SPIE Photonics West, **San Francisco, CA (USA),** 23–28, Jan 2010 (Oral).

F. Sacconi, G. Romano, G. Penazzi, M. Povolotskyi, M. Auf der Maur, A. Pecchia and A. Di Carlo. *Electronic and transport properties of GaN/ALGaN quantum dot based p-i-n diodes.* SISPAD 2008, **Hakone (Japan),** 9–11, Sep 2008 (Poster).

G. Romano, G. Penazzi, M. Auf der Maur, F. Sacconi, M. Povolotskyi, A. Pecchia and A. Di Carlo. *TiberCAD: the new multiscale simulator for electronic and optoelectronic devices*. 40th Electronic Group Meeting, **Otranto (Italy),** 16–18, Jun 2008 (Oral).

G. Romano, G. Penazzi, M. Auf der Maur, F. Sacconi, M. Povolotskyi, A. Pecchia and A. Di Carlo. *A new Multiscale simulator for electronics and optoelectronics devices.* New frontiers in micro and nanophotonics, **Florence (Italy),** 23–26, April 2008 (Oral).

G. Romano, M. Auf der Maur, M. Povolotskyi, F. Sacconi, E. Petrolati, A. Pecchia and A. Di Carlo. *Multiscale approach in the heat balance problems.* International summer school on advanced microelectronics, **Grenoble (France),** 24–29, Jun 2007 (Poster).

PROCEEDINGS

G. Romano, G. Penazzi and A. D. Carlo. Multiscale thermal modeling of GaN/AlGaN quantum dot LEDs. **Physics and Simulation of Optoelectronic Devices XVIII,** 7597(1), 75971S, SPIE (2010).

G. Penazzi, A. Pecchia, F. Sacconi, M. Auf der Maur, M. Povolotskyi, G. Romano and A. Di Carlo. *Simulations of Optical Properties of a GaN Quantum Dot Embedded in a AlGaN Nanocolumn within a Mixed FEM/atomistic Method.* **13th International Workshop on Computational Electronics** (IWCE ’09), 1 –4 (2009).

M. Auf der Maur, F. Sacconi, G. Penazzi, M. Povolotskyi, G. Romano, A. Pecchia and A. Di Carlo. *Coupling atomistic and finite element approaches for the simulation of optoelectronic devices.* **9th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD),** 75 – 80 (2009).

A. Di Carlo, M. Auf der Maur, F. Sacconi, A. Pecchia, M. Povolotskyi, G. Penazzi and G. Romano. *Multiscale atomistic simulations of high-k MOSFETs*. **Proceedings of the 8th IEEE International Conference on Nanotechnology** (2008).

A. Pecchia, G. Romano and A. Di Carlo. *Modeling of dissipative transport in molecular systems*. **Proceedings of the 7th IEEE International Conference on Nanotechnology,** 1185 – 1192 (2008).

F. Sacconi, G. Romano, G. Penazzi, M. Povolotskyi, M. Auf der Maur, A. Pecchia and A. Di Carlo. *Electronic and transport properties of GaN/AlGaN quantum dot-based p-in diodes*. **(SISPAD 2008),** 177 –180 (sept. 2008).

M. Auf der Maur, M. Povolotskyi, F. Sacconi, G. Romano, P. E. and A. Di Carlo. *Multiscale Simulation of Electronic and Optoelectronic Devices with TiberCAD.* **SISPAD 2007,** 245 –248 (sept. 2007).

JOURNAL ARTICLES (1/2)

G. Romano, A. Pecchia and A. Di Carlo. *Multiscale electro-thermal modeling og GaN/AlGaN quantum dot LEDs*. **IEEE Journal of quantum electronics,** (in preparation).

A. Gagliardi, G. Romano, A. Pecchia and A. Di Carlo. *Simulation of Inelastic Scattering in Molecular Junctions: Application to Inelastic Electron Tunneling Spectroscopy and Dissipation Effects.* **Journal of Computational and Theoretical Nanoscience** (in press).

M. Auf der Maur, F. Sacconi, G. Penazzi, M. Povolotskyi, G. Romano, A. Pecchia and A. Di Carlo. *Coupling atomistic and finite element approaches for the simulation of optoelectronic devices*. **Optical and Quantum Electronics** (in press).

G. Romano, A. Gagliardi, A. Pecchia and A. Di Carlo. *Heating and cooling mechanisms in single-molecule junctions*. **Physical Review B,** 81(11), 115438 (2010).

A. Gagliardi, G. Romano, A. Pecchia, A. Di Carlo, T. Frauenhe*Electron-phonon scattering in molecular electronics: From inelastic electron tunnelling spectroscopy to heating effects.* im and T. A. Niehaus. **New Journal of Physics,** 10 (2008).

G. Schulze, K. Franke, A. Gagliardi, G. Romano, C. Lin, A. Rosa, T. A. Niehaus, T. Frauenheim, A. Di Carlo, A. Pecchia and J. Pascual. *Resonant electron heating and molecular phonon cooling in single C60 junctions.* **Physical Review Letters,** 100(13) (2008).

JOURNAL ARTICLES (2/2)

A. Pecchia, G. Romano, A. Di Carlo, A. Gagliardi and T. Frauenheim. *Joule heating in molecular tunnel junctions: Application to C60.* **Journal of Computational Electronics,** 7(3), 384 – 389 (2008).

M. Auf Der Maur, M. Povolotskyi, F. Sacconi, A. Pecchia, G. Romano, G. Penazzi and A. Di Carlo. *TiberCAD: Towards multiscale simulation of optoelectronic devices*. **Optical and Quantum Electronics,** 40(14-15 SPEC. ISS.), 1077 – 1083 (2008).

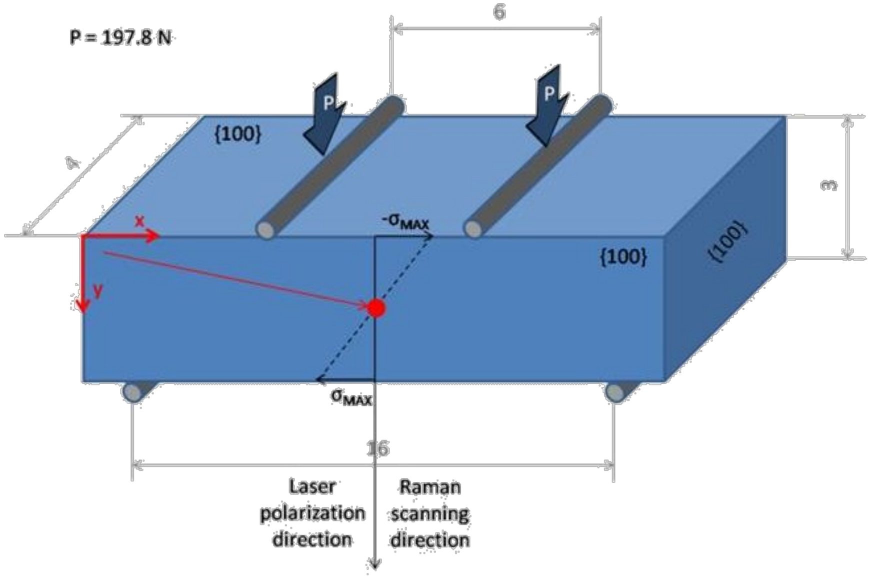
G. Romano, A. Pecchia and A. Di Carlo. Coupling of molecular vibrons with contact phonon reservoirs. **Journal of Physics Condensed Matter,** 19(21) (2007).

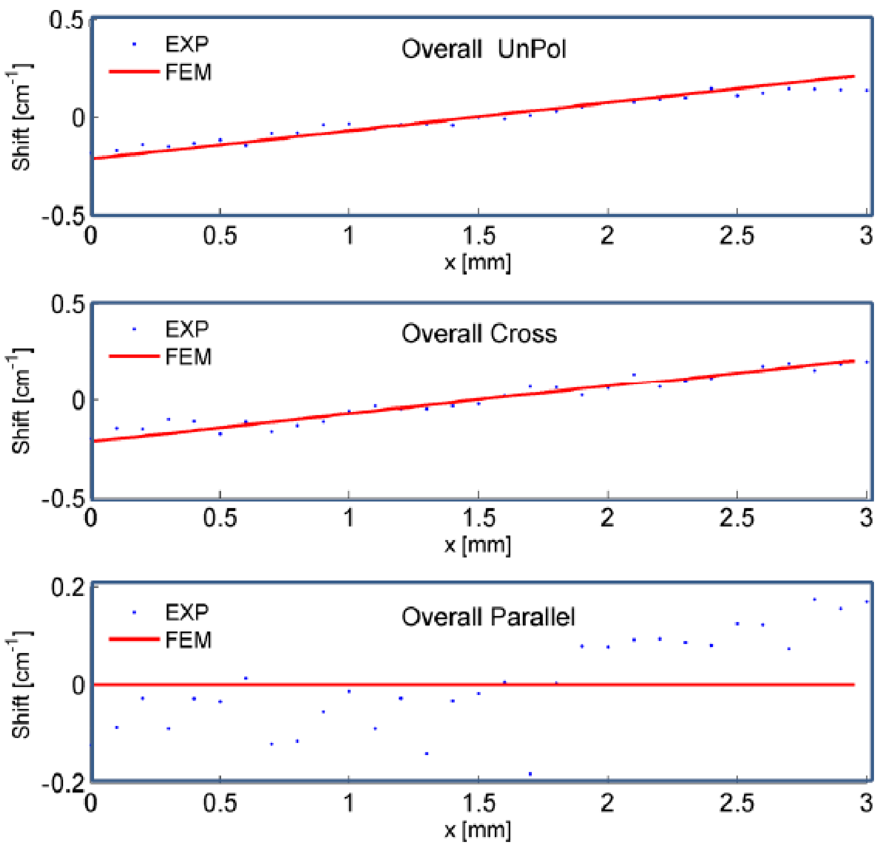
A. Pecchia, G. Romano and A. Di Carlo. Theory of heat dissipation in molecular electronics. **Physical Review B,** 75(3), 35401 – 1 (2007).

A. Pecchia, G. Romano, A. Gagliardi, T. Frauenheim and A. Di Carlo. Heat dissipation and non-equilibrium phonon distributions in molecular devices. **Journal of Computational Electronics,** 6(1-3), 335 – 339 (2007).

Kyoto Institute of Technology, Kyoto (Japan) Aug-Oct 2008

Theoretical piezospectroscopic



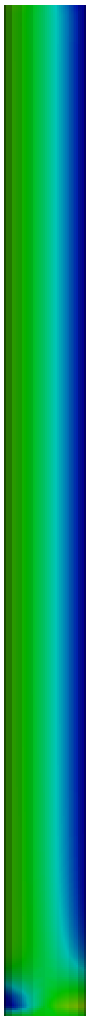


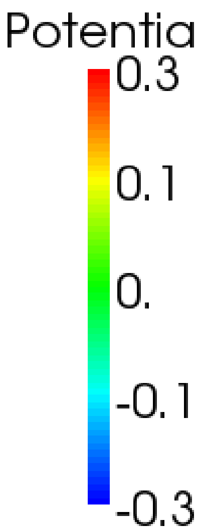
Deformation potentials

Raman shift

Prof. Giuseppe Pezzotti

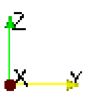
Georgia Institute of Technolgy, Atlanta, GA (Aug-Oct 2009)



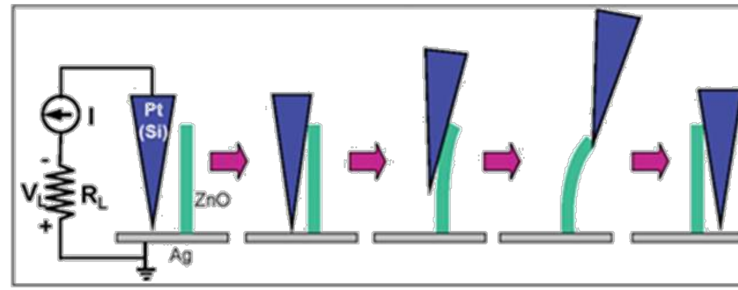


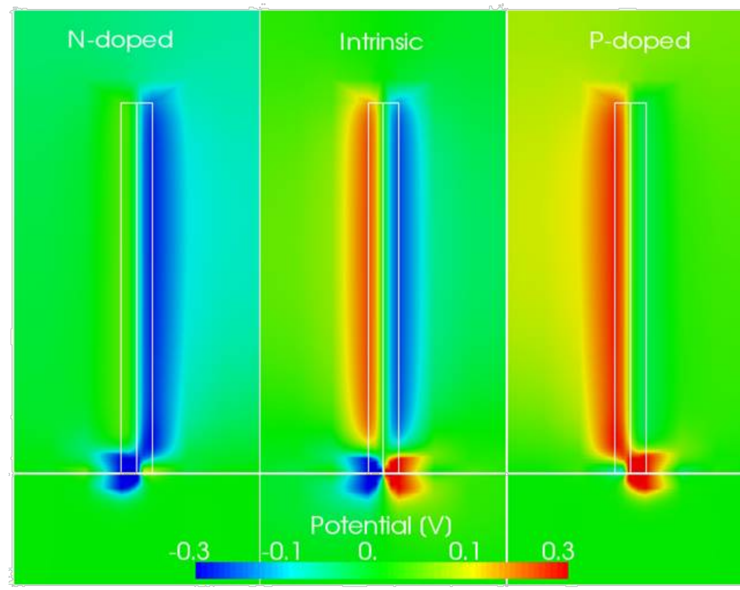
$V^{-}_{max} \approx 0.3\ V$

$V^{+}_{max} < 0.05\ V$



$z_0 = 300\ nm$





Prof. Zhong Lin Wang