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Laboratoire d'Excellence en Nanosciences et Nanotechnologies

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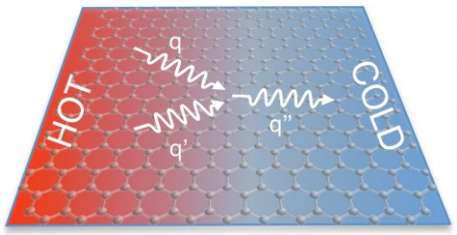
SCIENTIFIC REPORT for the WORKSHOP

Advanced thermoelectrics at nanoscale: from materials to devices



July 07, 2015 - July 10, 2015
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1 Summary and Discussion

State of the art Thermoelectric nanomaterials, whose combination of thermal, electrical, and semiconducting properties allows them to convert heat into electricity, are expected to play an increasingly important role in meeting the energy challenge of the future. Major advances in this field strongly depend on our fundamental understanding of heat and charge carrier transport and on the ability of finding new strategies to design and fabricate high efficiency thermoelectric devices and circuits. Despite of the substantial advances in the description of thermal and electronic dynamics in bulk materials, the extension of transport bulk theory to nanostructures, is still under development. One of the main problems in modeling the nanostructures for thermoelectrics is the fact that they usually have complex compositions and structures. To these complex structures, usually, several external elements are added to improve either the thermoelectric properties and to become functional elements of devices and circuits. The final material is hence a quite complex object whose phononic and electronic structure is unknown.
Recently it is starting to be a widespread belief among the research community that more accurate theories and approaches are needed. In particular first-principles calculations (i.e. accurate simulations free of adjustable parameters like Density Functional Theory and Density Functional Perturbation Theory) have started to be considered the most reliable way of computing phonons and electrons related quantities in a material. Usually these kinds of simulations are combined with quantum (i.e. Non equilibrium Green's Functions), semi-classical (i.e. Boltzmann Transport Theory) or classical (i.e. Molecular Dynamics) approaches in order to get electronic and thermal conductance and to take into account specific effects (i.e. when different types of scattering or bigger systems have to be considered). Very recently also the coupling of the above-mentioned methods with macroscale approaches (e.g. compact models) has emerged a promising way to reproduce devices and circuit characteristics through modeling. In all these hierarchical multiscale strategies one carries out the computational simulation at one scale and extracts such quantities that can be used to define the parameters of the model operative on the adjoining (usually larger) scale.

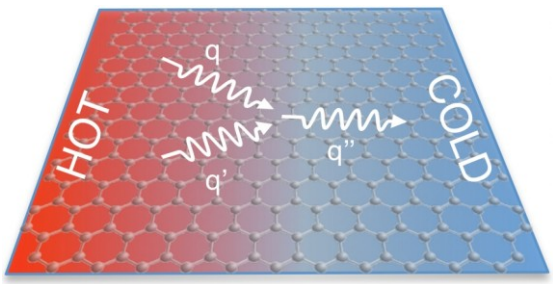

Figure 1 Pictorial view of phonon scattering in graphene [from Fugallo et al., Nano Lett., 14 (11), pp 6109 (2104)]. Two talks of the workshop discussed the role of collective vs single phonon excitations, one of the most exciting recent developments in the theory of nanoscale thermal transport.

Outlook: where is the field going? Despite thermoelectricity is still largely governed by engineering sectors, that favours an empirical approach to the problems, rather pursuing a fundamental understanding of the underlying physics, encouraging signals are coming from basic research. We foresee an increasingly important role of theoretical modelling and simulations in what, rather than application oriented, we would like to name application inspired research. The key challenge for the next 3-5 years is creating a real synergy with industrial R&D divisions. For his to happen, modelling must become more

predictive, on oine hand, must be able to communicate that its predictive capability, rather than quantitative, can be qualitative (elucidation of trends, highlighting of physical mechanisms) and still be useful.

Major obstacles to success As detailed in the state-of-the-art section above, systems that are candidates to be efficient thermoelectric materials are intrinsically complicated for what their (nano) structure and chemical composition are concerned. Multiscale modelling is a possible way out of this conundrum and we believe that additional research efforts in this direction should be made.

Novelty in workshop organization We have introduced a novelty in the traditional CECAM workshop program by inviting a world leader in the field of thermoelectricity, prof. Mark Lundstrom (Purdue University) to give a tutorial lecture. Prof. Lundstrom is author of several seminal papers and a bestselling book on nanoscale electron transport. We invited him with the specific task of delivering the opening lecture of the workshop with a deliberate tutorial flavor. At variance with ordinary invited talks of the workshop we reserved a 1h30' slot for this inaugural talk. We must say that, not only students, but also senior scientists were delighted by the pedagogical character of such introductory lecture. We firmly believe that, when possible, this should be a standard in every CECAM workshops and certainly will be in those that we might organize in the future.
Another minor novelty, already implemented by a few workshops in the past, is that we are collecting the presentations of all the speakers that has given their consent in this direction, and will upload them on the workshop website for dissemination. We believe that, especially in the case of tutorial presentations like the one of Prof. Lundstrom, this can gather a considerable interest.

Funding It would be unfair saying that the field of thermoelectricity has not previously received funding from the regular programs of the EU. However, we strongly believe that this is the right time for a strategic increase of funding in this area. As said, modelling can be of great utility, but has been too often neglected in these large-scale projects. Specific calls directed to the theoretical community could partially restore this unbalance.

Industrial and Societal interest In the documents describing the specific programme implementing Horizon 2020 it is explained that the specific programme shall consist of the following parts: (a) Part I *Excellent science*; (b) Part II *Industrial leadership*; (c) Part III *Societal challenges*; (d) Part IV *Non-nuclear direct actions of the Joint Research Centre* (JRC).
The output of the workshop is directly linked with *Excellent science*, *Societal challenges*, and indirectly with *Industrial leadership*.
PART I *Excellent Science* employs the following schemes to promote research on enabling technologies:
- European Research Council
- Future and Emerging Technologies (FET Open, FET Proactive)
- Marie Curie actions
- Research Infrastructures

An output of our workshop is that a clear focus on collaborative research projects entirely or at least partially based on ab-initio calculations is a necessary choice since more and more it is necessary to understand the properties of new materials at the nanoscale, at atomistic level in order to guide the experimental work towards innovation.
PART II *Industrial leadership* within Horizon 2020 shall strengthen industrial leadership by pursuing the following specific objectives:
"Boosting Europe's industrial leadership through research, technological development, demonstration and innovation in the following enabling and industrial technologies: (i)

Information and communication technologies; (ii) Nanotechnologies; (iii) Advanced materials."

The envisaged introduction of new nanomaterials for thermoelectric application play an important role in both items (i) and (ii) assuring at the same time a possible Europe's industrial leadership in this field.

PART III *Societal challenges* shall contribute to Horizon 2020 by pursuing research, technological development, demonstration and innovation actions which contribute, among others, to the following specific objectives:

"Making the transition to a reliable, sustainable and competitive energy system, in the face of increasing resource scarcity, increasing energy needs and climate change;"

In particular, regarding the priority Secure, clean and efficient energy we envisage two main important points in favor of nanostructured thermoelectric materials and devices, i) In thermoelectric application, where reliable and scalable, devices are presently used in a number of applications for both turning heat into electricity, measuring temperature and using electricity to produce cooling (Peltier cooling and temperature controllers). For the design of practical energy generator devices, not only the efficiency has to be taken into account. Indeed, since the waste heat is abundant (and of course inevitable) in industrial processes, home heating and automotive exhaust, the specific output power, which in the end determines the final utilization of the generated power, turns to be more significant. Thus nanostructured based devices assumed a special importance since the have low cost and can be fully integrated, (ii) the substitution of rare and toxic material, one of the main action that Europe will favor in Horizon 2020.

2 Program

Day 1 - Tuesday July 7, 2015

Registration and welcome

- 8:30 to 8:50 – Registration
- 8:50 to 9:00 – Welcome

Opening lecture

- 9:00 to 10:30 - **Mark S. Lundstrom**
  Electrothermal transport: from electrons to phonons
- 10:30 to 11:00 – Coffee Break

Fundamental theory of thermoelectrics

- 11:00 to 11:40 - **Massimiliano Di Ventra**
  Functional theories of thermoelectric phenomena
- 11:40 to 12:00 - **Christophe Goupil**
  When thermoelectric systems meet the Feymann ratchet: harmonic response and feedback
- 12:00 to 12:40 - **Yann Chalopin**
  Statistical approaches of phonon transport in nanostructures: toward novel characteristic length scales in radiation and conduction
- 12:40 to 14:10 – Lunch
- 14:10 to 15:00 - **Giuliano Benenti**
  Fundamental aspects of steady state heat to work conversion

Bulk thermoelectric materials I

- 15:00 to 15:40 - **Yee Kan Koh**
  The role of Akhieser's damping in the heat conduction by phonons with long mean-free-paths in silicon
- 15:40 to 16:00 - **Ming Hu**
  Anomalous pressure dependent lattice thermal conductivity of bulk thermoelectric materials: a first-principles study
- 16:00 to 16:20 - **Kristian Berland**
  The role of the exchange account in density functional theory calculations of thermoelectric properties
- 16:20 to 17:00 – Coffee Break
- 17:00 to 17:40 - **Joo-Hyoung Lee**
  Computational Design of high-performance thermoelectric materials

- 17:40 to 18:20 - **Alejandro Goñi**
  Polymer/carbon nanotube composites with positive-to-negative tunable Seebeck coefficient

Welcome cocktail

- 19:00 to 20:00 – Cold buffet

Day 2 - Wednesday July 8, 2015

Graphene-based materials

- 9:00 to 9:40 - **Giorgia Fugallo**
  Thermal properties of graphene and related compounds from first-principles

- 9:40 to 10:20 - **Claudio Melis**
  Thermal transport in graphene-based systems for thermoelectric applications

- 10:20 to 11:00 – Coffee Break

- 11:00 to 11:40 - **Andrea Cepellotti**
  Phonon hydrodynamics in two-dimensional materials

- 11:40 to 12:00 - **Giuliana Barbarino**
  Hydrogenation as a novel perspective for thermal rectification in graphene nanoribbons

- 12:00 to 14:00 – Lunch

Si-based materials

- 14:00 to 14:40 - **Clivia M. Sotomayor Torres**
  Thermal transport in free-standing silicon membranes

- 14:40 to 15:00 - **Daniele Selli**
  Improved thermoelectric features in low dimensional silicon based devices

- 15:00 to 15:40 - **Armando Rastelli**
  Thermal and thermoelectric transport through Ge/Si multilayers

- 15:40 to 16:20 – Coffee Break

Molecular junctions

- 16:20 to 17:00 - **Kristian Thygesen**
  First-principles GW calculations of conductance and thermopower of molecular junctions

- 17:00 to 17:20 - **Carmine Antonio Perroni**
  Thermoelectric efficiency of molecular junctions

- 17:20 to 17:40 - **Falco Hüser**
  From chemistry to functionality: length dependence of thermopower in molecular junctions

Day 3 - Thursday July 9, 2015

Nanowires

- 9:00 to 9:40 - **Renkun Chen**
  Thermal and thermoelectric transport in thin semiconductor nanowires

- 9:40 to 10:00 - **Konstantinos Termentzidis**
  Amorphous/crystalline superlattices and nanowires for thermoelectric applications

- 10:00 to 10:20 - **Milo Swinkels**
  Diameter dependent thermal conductivity of single InAs nanowires for thermoelectric applications

- 10:20 to 11:00 – Coffee Break

- 11:00 to 11:40 - **Byoung Lyong Choi**
  Phonon scattering enhancement from Si-based nanowires for large thermoelectric figure-of-merits

- 11:40 to 12:00 - **Stefano Roddaro**
  Complete thermoelectric benchmarking of individual InSb nanowires by combined micro-Raman and transport analysis

- 12:00 to 14:00 – Lunch

Bulk thermoelectric materials II

- 14:00 to 14:40 - **Jelena Sjakste**
  Electron-phonon and phonon-phonon coupling in semiconductors and bismuth: theoretical approaches

- 14:40 to 15:00 - **Yongjin Lee**
  Fundamental insight and control into heat transport in silicon-based alloy systems

- 15:00 to 19:45 – Day off

Social dinner

- 19:45 to 23:00 – Dinner cruise

Day 4 - Friday July 10, 2015

Molecular Dynamics and Multiscale simulations

- 9:20 to 10:00 - **Alan McGaughey**
  Vibrational mode properties in disordered solids

- 10:00 to 10:20 - **Jérôme Saint-Martin**
  Multiscale modelling of thermoelectrics generators based on graphene nanostructures

- 10:20 to 11:00 – Coffee break

- 11:00 to 11:20 - **Theodoros Karakasidis**
  A multiscale approach for the calculation of transport properties of liquids

- 11:20 to 12:00 - **Che-Wun Hong**
  Thermoelectric chip design simulation and EV applications: from quantum mechanics to system dynamics

- 12:00 to 12:15 – Closing Word

- 12:15 to 14:00 – Lunch

3 Abstracts

Electrothermal transport: from electrons to phonons

Mark S. Lundstrom[1], Jesse Maassen[1]
[1]School of Electrical and Computer Engineering, Purdue University, USA

The field of electron transport in semiconductors has developed, evolved, and matured alongside the development of semiconductor technology from microelectronics to nanoelectronics. It began with van Roosbroeck's classic formulation of the semiconductor equations (drift-diffusion) in 1950, continued with the development of Monte Carlo techniques to solve the Boltzmann equation for electrons in the 1960's, and has resulted today in the widespread simulation of electron transport with the non-equilibrium Green's function (NEGF) approach. As microelectronics transitioned to nanoelectronics in the 1990's, elegant experiments complemented by insightful analyses led to a clear, deep understanding of mesoscopic transport. We now understand transport from ballistic to diffusive conditions, what electrochemical potentials in nanostructures mean, where the voltage drops occur, etc. The field of thermal transport has an even longer history beginning with Fourier's Law, to the numerical solutions of phonon Boltzmann equation, to today's sophisticated molecular dynamics simulations. But electrons and phonons always go together – sometimes it is a problem, as in the self-heating of electronic devices, and sometimes it is the whole point, as in thermoelectrics. Our goal in this talk is to encourage a dialogue between experts in electron and phonon transport and to think about whether there is a set of concepts and tools that can help us better understand and analyze electron and phonon transport together. This talk will present an electron transport perspective on thermal transport. Our goal is to discuss the remarkably simple conceptual picture of electron transport at the nanoscale that has emerged from decades of work on experiments and sophisticated transport theory and simulations and to explore its application to thermal transport. The two central concepts are the Landauer approach, which provides a connection to both semiclassical (Boltzmann) and quantum (NEGF) transport and the McKelvey-Shockley one-flux form of the Boltzmann equation. We'll discuss the similarities and differences of electron and phonon transport and some new insights into thermal transport that come from using concepts from electronics. One example is the fact that Fourier's Law often works extremely well at that nanoscale. We will show results that suggest that the techniques developed for electron transport can be useful in heat transport as well. Finally, I'll try to identify some issues that need to be addressed if we are to develop a comprehensive conceptual and computational framework for electrothermal transport.

Functional theories of thermoelectric phenomena

Massimiliano Di Ventra[1]
[1]University of California, San Diego, USA

I will discuss non-equilibrium density functional theories of local temperatures and associated heat currents that are particularly suited for the study of thermoelectric phenomena. In one case, I will introduce a functional theory of open quantum systems [1] that allows the study of local temperatures by the introduction of local thermal probes. In another [2], we couple the local temperature field to an energy density operator. I will also provide predictions on the local temperature oscillations in atomic wires [3], carbon nano-ribbons and graphene junctions [4], and discuss similarities and differences between the different local temperature definitions in the strongly-correlated regime [5].

[1] M.Di Ventra and R. D' Agosta, Phys. Rev. Lett. 98, 226403 (2007).
[2] F. Eich, G. Vignale and M. Di Ventra, Phys. Rev. Lett. 112, 196401 (2014).
[3] Y. Dubi and M. Di Ventra, Nano Lett. 9, 97 (2008).
[4] J.P. Bergfield, M. A. Ratner, C. A. Stafford, and M. Di Ventra, arXiv: 1305.6602
[5] L.Z. Ye, D. Hou, X. Zheng, Y.J. Yan, and M. Di Ventra, in preparation.

When thermoelectric systems meet the Feymann ratchet: harmonic response and feedback

Christophe Goupil[1], Yann Apertet[2], Henni Ouerdane[2], Philippe Lecoeur [2]
[1]Laboratoire Interdisciplinaire des Energies de Demain, Université Paris Diderot, Paris
[2]Institut d'Electronique Fondamentale, Université Paris-Sud, Orsay, France

In his reflections on the motive power of heat, Carnot established that heat-to-work conversion is a process that only occurs with a limited efficiency. More than a century later, Feynman, in his Lectures on Physics, thought it was worthwhile to provide a physically transparent explanation of this limitation, basing his analysis on elementary mechanical arguments. The simplest mechanical device that could serve this purpose was that which allows a shaft to rotate only one way to transmit motion: the ratchet and pawl system, originally designed by Smoluchowski and known nowadays as a Brownian or Feynman ratchet. Using this system as a bridge from macroscopic to mesoscopic physic we propose to revisit the description of the thermoelectric devices and its extension to the non stationary response. In particular we show that the presence of a feedback from the output electrical power to the input heat power introduces some extra terms to the dissipation and the dynamical response.

Statistical approaches of phonon transport in nanostructures: toward novel characteristic length scales in radiation and conduction

Yann Chalopin[1]
[1]Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion, École Centrale Paris, Châtenay Malabry, France

The aim of this talk is to introduce an atomistic description of thermal transport from a unified approach which is based on microscopic correlations. We will mostly discuss the radiative and conductive properties of different classes of nano-materials (semiconductors, oxides, soft-matter…) by demonstrating that novel thermal properties of matter can be investigated by tracking the momentum and displacement fluctuations of atomic nucleus. The outline of the presentation is constructed in three parts: The first discusses infrared absorption in dielectric nano-objects and the violation of the classical electrodynamics at specific length scales. The next part introduces the Kapitza problem and the spectral decomposition of the thermal conductance at solid:solid but also solid:fluid interfaces. Finally, we present an estimator -so-called the coherence length - which unveils the particle versus wave nature of the phonons and consequently allows tailoring thermal properties of matter with an original and novel approach.

Fundamental aspects of steady state heat to work conversion

Giuliano Benenti[1]
[1]Università degli Studi dell'Insubria, Como, Italy

The understanding of coupled charge and heat transport in complex systems is a fundamental problem, also of practical interest in connection with the challenging task of developing high-performance thermoelectric heat engines and refrigerators, the low efficiency of existing thermoelectric devices being the factor which limits their use. To investigate this problem, we follow an approach which starts from first principles i.e. from the fundamental microscopic dynamical mechanisms which determine the phenomenological laws of heat and particle transport. We compute the basic transport coefficients (isothermal charge conductivity, heat conductivity, thermopower, and Peltier coefficient) starting from the microscopic equations of motion of stylized models, including billiard models and single- or few-level quantum dots. The transport coefficients are computed by means of nonequilibrium simulations (stochastic reservoirs) and the Green-Kubo formula in classical models, while the (multi-terminal) Landauer-Buttiker approach is used for non-interacting quantum systems. We show that for systems with a single relevant constant of motion, notably momentum conservation, the thermoelectric efficiency reaches the Carnot efficiency in the thermodynamic limit [1]. Such general result is illustrated by means of numerical simulations in the case of a diatomic chain of hard-point elastically colliding particles [1] as well as for Coulomb interaction [2] and for a two-dimensional gas of interacting particles [3]. For systems with broken time-reversal symmetry,

we show [4] that the maximum efficiency and the efficiency at maximum power are both determined by two parameters: a generalized figure of merit and an asymmetry parameter, given by the ratio of the thermopowers obtained for opposite directions of the magnetic field [4-6]. In contrast to the time-symmetric case, the figure of merit is bounded from above; nevertheless the Carnot efficiency can be reached at lower and lower values of the figure of merit and far from the so-called strong coupling condition as the asymmetry parameter increases. Moreover, the Curzon-Ahlborn limit for efficiency at maximum power can be overcome within linear response, as we have shown numerically in a few examples (Aharonov-Bohm interferometer formed with three non-interacting quantum dots, transmission windows model) [7]. Finally, always within linear response, it is not forbidden by the laws of thermodynamics to have Carnot efficiency and non zero power simultaneously [4]. We also discuss the efficiency of a thermal engine working in linear response regime in a multi-terminal configuration [8]. We provide a general definition of local and non-local transport coefficients (electrical and thermal conductance, and thermoelectric powers). Within the Onsager formalism and in the three-terminal case, we derive analytical expressions for the efficiency at maximum power, which can be written in terms of generalized figures of merit. Also, using two examples (single and double dot), we investigate numerically how a third terminal could improve the performance of a quantum system, and under which conditions non-local thermoelectric effects can be observed. Finally, we show that three-terminal configurations allow heat-charge separation favorable for thermoelectric conversion [9] and, in presence of a magnetic field, the design of thermal switches [10].

[1] G. Benenti, G. Casati, and W. Jiao, Phys. Rev. Lett. 110, 070604 (2013).
[2] S. Chen, W. Jiao, G. Casati, and G. Benenti, "Thermoelectric efficiency in Coulomb gas model", preprint.
[3] G. Benenti, G. Casati, and C. Mejia-Monasterio, New J. Phys. 16, 015014 (2014).
[4] G. Benenti, K. Saito, and G. Casati, Phys. Rev. Lett. 106, 230602 (2011).
[5] K. Saito, G. Benenti, G. Casati, and T. Prosen, Phys. Rev. B 84, 201306(R) (2011).
[6] M. Horvat, T. Prosen, G. Benenti, and G. Casati, Phys. Rev. E 86, 052102 (2012).
[7] V. Balachandran, G. Benenti, and G. Casati, Phys. Rev. B 87, 165419 (2013).
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[9] F. Mazza, S. Valentini, R. Bosisio, G. Benenti, V. Giovannetti, R. Fazio, and F. Taddei, "Separation of heat and charge currents for boosted thermoelectric conversion", preprint.
[10] R. Bosisio, S. Valentini, F. Mazza, G. Benenti, V. Giovannetti, R. Fazio, and F. Taddei, "A magnetic thermal switch for heat management at the nanoscale", preprint.

The role of Akhieser's damping in the heat conduction by phonons with long mean-free-paths in silicon

Yee Kan Koh[1], Puqing Jiang[1]
[1]Department of Mechanical Engineering, National University of Singapore, Singapore

Despite recent progress in first-principles calculations and measurements of the mean-free-paths of phonons, contribution of phonons with long mean-free-paths to heat conduction in silicon is still inconclusive. For example, first-principles calculations by Broido et al. suggest that phonons with mean-free-path > 1 μm contribute ~45% to the thermal conductivity of silicon at 300 K, but the calculations by Garg et al. show that the contribution is only ~25%. Moreover, appreciable reduction in the thermal conductivity was not observed in prior measurements of the in-plane thermal conductivity of micron-sized silicon thin films. In this talk, we will report our recent experimental results to determine the contribution of phonons with mean-free-paths > 1 μm, by accurately measuring the in-plane and cross-plane thermal conductivities of a wide range of crystalline silicon films with a thickness of 1-10 μm at temperatures of 100-300 K by time-domain thermoreflectance (TDTR). We employ a dual-frequency TDTR approach in our cross-plane thermal conductivity measurements to improve the accuracy. Our measurements fall between predictions derived from the first-principles calculations by Garg et al. and by Broido et al. Using a model that includes Akhieser's damping for low-energy phonons, we estimate that inclusion of Akhieser's damping reduces the calculated thermal conductivity of silicon by ~9% and thus provides a possible explanation for the discrepancy between our measurements and the first-principles calculations. Our work provides important benchmarks for future measurements and calculations of the distribution of phonon mean-free-paths in crystalline silicon.

Anomalous pressure dependent lattice thermal conductivity of bulk thermoelectric materials: a first-principles study

Ming Hu[1,2], Tao Ouyang[1]
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[2]Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen University, Germany

Pressure tuning and exploration of high pressure phase are effective approaches to modulate the electronic properties and optimize the thermoelectric performance. For example, the researchers found that pressure can significantly improve the power factor of some thermoelectric materials, e.g. PbTe, Bi_2Te_3 and Sb_2Te_3. The high pressure phase of PbTe and HgTe are also predicted to possess super thermoelectric efficiency. However, in these works the phononic thermal conductivity is simply estimated by the Wiedemann-Franz relation or assumed to be the same value for all different phases, which give rise to the inaccuracy of thermoelectric performance. In order to predict the thermoelectric property more accurately, it is desirable to investigate the lattice thermal transport through first-principles-based approach. In this work, based on first-principles calculations we find a surprising decrease in lattice thermal conductivity with pressure for some promising thermoelectric materials, which originates from the anomalous increase in anharmonic phonon scattering induced by the compression. Our first-principles calculations reveal that, comparing with typical bulk materials like diamond, the unique electron distribution in some thermoelectric materials results in low shear modulus and strong anharmonic phonon scattering. With applied pressure, the anharmonicity of such materials is further enhanced and thus drives the lattice thermal conductivity to low values. We also find that there is always a completion between the enhancement of longitudinal acoustic modes which facilitates thermal transport and the depression of transverse acoustic modes which hinders the heat transfer. Our findings change our common understanding that lattice thermal conductivity of bulk materials always increases upon compression and offer a new route for advancing the energy conversion performance of thermoelectric materials.

The role of the exchange account in density functional theory calculations of thermoelectric properties

Kristian Berland[1], Clas Persson[1]
[1]University of Oslo, Norway

With ongoing efforts to better account for electronic scattering mechanisms in ab-initio based approaches, we can expect more accurate theoretical predictions of thermoelectric properties such as the Seebeck coefficient. This expectation motivates our study of how these properties are impacted by the choice of the exchange functional used in density-functional theory (DFT) calculation of the band structure. With traditional functionals such as PBE, band gaps are often underestimated, while hybrid exchange functional such as HSE is typically more accurate. Studying a set of bulk thermoelectric materials, we find that for some materials, this issue is ameliorated by widening the band gap by hand, whereas for other ones, HSE drastically alters the shape of the density of states and thus computed thermoelectric properties.

Computational design of high-performance thermoelectric materials

Joo-Hyoung Lee[1]
[1]Gwangju Institute of Science and Technology, South Korea

As the world's demand for energy rapidly increases while fossil fuel supplies decrease, it is becoming more important to develop new, inexpensive materials that can supply sustainable and clean energy to meet the needs of the future. One of promising approaches in this direction relies on thermoelectric (TE) materials, which convert temperature gradient directly into electricity. While traditional TE materials such as Bi_2Te_3 have witnessed applications over decades, they contain expensive, rare, heavy and sometimes harmful elements. It is thus crucial to search for novel and abundant materials and/or structures with a view towards high efficiency, cost-effective energy conversion applications. Notably, recent advances in semiconductor nanostructures have

provided a new strategy along this direction. In this talk, I will describe how state-of-the-art computational approaches can play an important role in designing high-performance TE materials using crystalline Si and II-VI semiconductors, by providing both fundamental understanding on the conversion properties of these materials and guidance for their experimental synthesis. Since it is critical to understand the thermal and electronic properties of a material in order to develop efficient TE devices, emphasis will be given to how our understanding of these properties can be advanced through computational approaches.

Polymer/carbon nanotube composites with positive-to-negative tunable Seebeck coefficient

Alejandro Goñi[1], Bernhard Dörling[1], C. Bounioux[3], Jason Ryan[4], Matthew C. Weisenberger[5], Andrea Sorrentino[6], Ahmed El Basati[1], Miquel Garriga[1], Eva Pereiro[6], Rachel Yerushalmi-Rozen[3], John E. Anthony[5], Christian Müller[4], Mariano Campoy-Quiles[1]
[1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Bellaterra, Spain
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Conjugated polymers are receiving renewed attention for thermoelectric applications as they readily offer the desired ease of processing from solution, which enables printing on large-area, flexible substrates. An additional advantage is the low thermal conductivity (0.1–0.5 $W \cdot m^{-1} \cdot K^{-1}$) of polymers. The two main strategies to increase the intrinsic thermoelectric properties of polymers, in particular, their relatively low electric conductivity, consist in controlling doping and fabrication of composites with high conducting fillers. Here we combine the two strategies to make composite films of doped poly(3-hexylthiophene) and carbon nanotubes (CNTs) that offer a competitive thermoelectric performance. The power factor significantly exceeds values obtained with either constituent alone provided that the conjugated polymer is sufficiently p-doped. The use of single-walled CNTs consistently results in a higher electrical conductivity than multi-walled CNTs with a maximum value in excess of 103 S/cm, which gives rise to a power factor close to 100 $\mu W \cdot m^{-1} \cdot K^{-2}$ for 42–81 wt%. Moreover, a carbon nanotube content of 8–10 wt% does not compromise the low bulk thermal conductivity of the polymer matrix, which promises a high figure of merit ZT around 0.2 at room temperature. All samples are cast on plastic substrates, emphasizing their suitability for large-area, flexible thermoelectric applications. Finally, we also present new results of experiments conducted on composites of P3HT and nitrogen-doped multi-walled carbon nanotubes (n-doped MWCNTs) [2]. The striking property of these composites is that they show both p-type and n-type behavior, depending on the mixing ratio and preparation protocol. For low CNT content, the Seebeck coefficient is positive, as is expected for P3HT. Increasing the CNT content decreases the Seebeck coefficient into negative values. The resulting power factor has two maxima, one near 20 wt% CNT content, where the composite shows positive Seebeck, and another near 80 wt% CNTs, where it acts as n-type thermoelectric material. We illustrate the potential of the developed technology by showing two working flexible thermoelectric generator prototypes.

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Thermal properties of graphene and related compounds from first-principles

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In recent years heat removals has become one of the crucial issue for continuing progress in the

electronic industry, and thermal conduction in 2D systems, especially graphene, has revealed truly intriguing and promising features [1-3]. I will present here a fully first principle characterization of the thermal conductivity of graphite, monolayer graphene, graphane, fluorographane, and bilayer graphene obtained by solving exactly the Boltzmann transport equation for phonons [4]. For graphite, the results are found to be in excellent agreement with experiments; notably, the thermal conductivity is one order of magnitude larger than what found by solving the Boltzmann equation in the single mode approximation, commonly used to describe heat transport. For graphene, I will point out that 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. This unusual requirement is due to the fact that collective phonon excitations, and not single phonons, are the main heat carriers in these materials; and these excitations are characterized by mean free paths of the order of hundreds of micrometers [5]. As a result, even Fourier's law, due to its statistical nature, becomes questionable in typical sample sizes.

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Thermal transport in graphene-based systems for thermoelectric applications

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Graphene has been recently indicated as a promising material for several energy applications such as photovoltaics, fuel cells and many others [1]. Among them, one of the most promising applications of graphene is thermoelectricity i.e. devices that generate electricity from a temperature gradient. However, graphene has both high electric and thermal conductivity, a combination not ideal for thermoelectric devices. A possible way of increasing graphene's thermoelectic figure of merit is to tailor its thermal transport properties by several nano-structuring techniques. In this seminar I will address such a perspective by focusing on graphene lattice thermal conductivity by means of non-equilibrium molecular dynamics simulations, and provide the following information: • Intrinsic thermal conductivity in monolayer graphene is ultimately upper limited [2] • nanostructuration [3] and hydrogenation [4] are two possible ways of reducing graphene thermal conductivity • a proof of concept investigation of graphene-based thermal rectifiers [5].

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Phonon hydrodynamics in two-dimensional materials

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Heat conduction of materials is a fascinating property, which achieves its highest values in 2D crystals [1], although the microscopic nature of the phonon transport mechanisms in systems of reduced dimensionality remains largely obscure. Here we use density-functional perturbation theory and an exact, variational solution of the Boltzmann transport equation [2] to study fully from first-principles phonon transport and heat conductivity in 2D materials. In all these systems, and at variance with typical three-dimensional materials, normal (heat-flux conserving) processes keep dominating over Umklapp scatterings well above cryogenic conditions, extending to room temperature and more [3]. As a result, the phonon gas behaves as an ideal fluid and novel

regimes emerge, with Poiseuille and Ziman hydrodynamics, hitherto typically confined to ultra-low temperatures, characterizing transport at ordinary conditions. Most remarkably, several of these two-dimensional materials admit wave-like heat transfer, in addition to ballistic and/or diffusive propagation, with second sound present at room temperature and above in graphene, boron nitride, and graphane.

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Hydrogenation as a novel perspective for thermal rectification in graphene nanoribbons

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We present a proof-of-concept molecular dynamics study in which we demonstrate that by suitably hydrogen decorating specific graphene nanoribbons it is possible to design a novel kind of thermal diodes. In particular, we estimate thermal rectifications at graphene/graphane interfaces with vertical, triangular and T-shaped morphology. We observe a significant thermal rectification in all cases achieving ~55% for the triangular graphene/graphane interface. The dependence of the thermal rectification on the nanoribbon dimensions and the temperature gradient is also explored. The physical origin of such an observed rectification is analyzed in terms of graphene/graphane interface thermal resistance and by comparing the heat current vector fields for forward and reverse polarizations. The present result is very promising for phononic applications were the control of the heat flux at the nanometer scale has been proposed as a perspective in designing novel switch-on-off devices as an alternative to conventional electronics.

Thermal transport in free-standing silicon membranes

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The model system offered by state-of-the-art free-standing ultra-thin silicon membranes [1] is used to study the contribution of acoustic phonons to the thermal conductivity in silicon with view to its applications as a thermoelectric material. Our understanding so far is based on measured and modeled acoustic phonon dispersion relations [2], their lifetime [3], the transport in the diffusive and ballistic regimes [4], the role of the native oxide [5], the role of 2-D phononic crystals in the membranes [6] and direct in-plane thermal conductivity measurements based on laser-Raman thermometry [7-8]. The dispersion relations of membranes of thickness down to 8 nm are measured and simulated and found to be discretised flexural and dilatational modes which deviations from the linear behavior close to q=0. The group velocity is obtained from these measurements and shown to decrease by a factor larger than 20. The lifetimes of the experimentally accessible first order dilatational mode is observed to decrease over one order of magnitude compared to bulk values. The data are used to model the thermal conductivity using a modified Akhieser mechanism incorporating the discrete and projected acoustic modes [9] and are compared to measurements based on thermal decay of a hot spot in the membranes. Boundary scattering and normal processes are found to contribute to the thermal transport as well as the native oxide. We will discuss our results in the light of thermodynamic models, non-equilibrium molecular dynamics calculations and the modified Akhieser approach modified to include the interplay of confinement and real surfaces and interfaces.

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Improved thermoelectric features in low dimensional silicon based devices

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Due to its relatively high thermal conductivity, bulk silicon is a poor thermoelectric material. However, its thermal conductivity can be reduced over two orders of magnitude by nanoscale engineering [1]. Recent advances in fabrication techniques, allow for the production of free-standing crystalline silicon membranes with varying thickness down to few nanometers [2]. By means of a combination of phononic and electronic theoretical investigations, we were able to characterize the thermoelectric performance of heavily phosphorous and arsenic doped silicon membranes in the ultra thin size domain. In order predict the total figure of merit of the membranes we made use of non-equilibrium Green's function formalism (NEGF) at a tight-binding level of theory [3] combined with a scattering matrix approach to evaluate the phononic thermal conductance [4]. Our results illustrate the concurrent effect of surface features (roughness, native silica) and dimensionality reduction in reducing the phononic thermal conductance and the consequences of doping on the Seebeck coefficient of the membranes. The two effects combined lead to a significant improvement of the thermoelectric figure of merit.

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Thermal and thermoelectric transport through Ge/Si multilayers

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We present experiments on epitaxial Ge/Si multilayers with cross-plane thermal conductivities which can be systematically varied by simply changing the thicknesses of the constituent layers. By performing the multilayer growth on Si(001) and Ge(001) substrates we investigate both Si- and Ge- rich multilayers. Ab initio calculations reveal that partial interdiffusion of Ge into the Si spacers, which naturally results from Ge segregation during growth, plays a determinant role, lowering the thermal conductivity below what could be achieved without interdiffusion, or with total interdiffusion (alloy limit). Our work suggests that superlattices with sharp interfaces, which are commonly sought but difficult to realize, are worse than compositionally-modulated $Si_{1-x}Ge_x$ multilayers in the search for materials with ultralow thermal conductivities. First results on in-plane thermal conductivity as well as cross- and in-plane electrical conductivity through the multilayers will be presented.

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First-principles GW calculations of conductance and thermopower of molecular junctions

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Molecular junctions in which one or several molecules are suspended between metallic electrodes represent a unique test-bed for advancing our understanding of charge, spin, and heat transport at the nano-scale. Molecular junctions can be seen as model systems that allow for detailed studies of charge transfer and energy level alignment at metal–molecule interfaces of relevance to, e.g., organic electronic devices and dye-sensitized solar cells. It has recently been proposed that molecular junctions could also be used as basis for thermoelectric energy conversion. As a first step towards this goal, several groups have recently reported measurements of the thermopower of various molecular junctions. In this context, thermopower measurements are also interesting as a spectroscopic tool as it provides information about the carrier type, i.e. whether the transport is dominated by the highest occupied molecular orbital (HOMO) or the lowest unoccupied molecular orbital (LUMO). Previous first-principles calculations of thermopower in molecular junctions have been based on density functional theory (DFT) within the Landauer formalism. While the standard generalized gradient approximation (GGA) to the exchange–correlation functional generally overestimates both thermopower and conductance better agreement with experimental values were reported for certain hybrid functionals with a simplified wideband approximations. Here we report on first-principles calculations of conductance and thermopower of molecular junctions treating the electron-electron interactions at the level of the many-body GW approximation. We show that the GW conductance and thermopower are significantly better agreement with experiments than those obtained from DFT for both p- and n-type junctions. The better performance of the GW approach is mainly a consequence of a better energy level alignment at the metal-molecule interface. However, dynamical screening effects, i.e. the fact that the screening in the metal contacts take place at a different time-scale than the tunneling time of the electron, also plays a role.

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Thermoelectric efficiency of molecular junctions

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The thermoelectric properties of a molecular junction model, appropriate for large molecules, are studied within a non-equilibrium adiabatic approach in the linear regime at room temperature. A self-consistent calculation is implemented for electron and phonon thermal conductance showing that both increase with the inclusion of the electron-vibration coupling [1]. Moreover, we show that the deviations from the Wiedemann-Franz law are progressively reduced upon increasing the interaction between electronic and vibrational degrees of freedom. Consequently, the junction thermoelectric efficiency is substantially reduced by the electron-vibration coupling. The adiabatic approach has been generalized to include large Coulomb repulsion through a self-consistent procedure [2]. We show that the phonon thermal conductance is quite sensitive to the effects of strong electron-electron interactions within the intermediate electron-vibration coupling regime bearing a strong resemblance with electron thermal conductance. In any case, the peak values of the thermoelectric figure of merit are of the order of unity for realistic values of junction parameters indicating that the emerging field of molecular thermoelectrics can be very interesting for applications.

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From chemistry to functionality: length dependence of thermopower in molecular junctions

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Potential materials for efficient thermoelectric devices are characterized by a high figure of merit, ZT.In this respect, organic molecules seem very promising candidates, due to their small size, high stability, easy fabrication and most of all, the vast number of possibilities of tuning their electrical and thermal properties. Ideally, one would like to predict a molecule's function from simple chemical trends. Yet, only little is known about the interplay between chemical structure and thermoelectric features like conductance or thermopower. Here, we present a systematic ab-initio study of the length dependence of the thermopower in molecular junctions. The molecules under consideration are small carbon chains with either saturated or fully conjugated backbones. They are attached to gold electrodes via a number of different binding groups in well defined contact geometries. Recent experiments [1] and tight-binding calculations [2] suggested that the thermopower depends linearly on the chain length. Based on a simple model for off-resonant tunneling, it has been stated that the offset (contact resistance) is given by the binding group, whereas the slope is determined by the molecular backbone. Our results, however, show that the story can be far more complicated. In particular, we find that gateway states can dominate the transport properties of the junction. Gateway states arise from hybridization of localized orbitals on the binding group with metal states of the electrodes. By investigating the electron transmission functions, we show how the presence, position and shape of resonances from these gateway states determine the length dependence of the thermopower. Different scenarios can be seen: positive and negative values for the contact thermopower and both increasing and decreasing behavior with length. This includes cases, where the thermopower changes sign for longer chains. Also, deviations from linearity are found. The results presented here were obtained with standard techniques based on Density Functional Theory and nonequilibrium Green's Functions for transport (NEGF-DFT). We discuss the validity and limits of this approach and compare to more sophisticated methods like self-energy corrections and the GW theory.

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Thermal and thermoelectric transport in thin semiconductor nanowires

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During the last decade or so we have witnessed tremendous advancement in the characterization and understanding of thermal transport in nanostructures, particularly in the ‘phonon boundary scattering’ regime where the characteristic size of nanostructures ranges from tens to hundreds nanometers and is comparable to phonon mean free path. This understanding is one of the key underlying reasons for improved performance observed in nanostructured thermoelectric materials. However, the boundary scattering mechanism may reach its limit and new mechanisms for improving thermoelectric performance need to be explored. One of the opportunities may arise from the study of thermal transport in the so-called ‘confinement’ regime, where the characteristic size of nanostructures is below 10-20 nanometers and is comparable to phonon wavelength. However, there is little experimental work on thermal transport in nanostructures in this regime. In this presentation, we will discuss our recent work on using rationally designed nanostructures to study nanoscale thermal and thermoelectric transport phenomena in this regime. We will describe the instrumentation we developed that enables the characterization of thermal transport and related properties of these nanostructures and discuss and interpret the measurement results.

Amorphous/crystalline superlattices and nanowires for thermoelectric applications

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Almost all silicon devices contain amorphous/crystalline interfaces and the transport for both electrons and phonons through them is a crucial issue. In this study, we model amorphous/crystalline interfaces for nanowires and superlattices. The aim is to predict the thermal conductivity and the phonon dispersion curves of these nanostructured materials. The calculations have been done with means of molecular dynamics simulations, with the use of realistic interatomic potential. The thermal conductivity of both nanostructures is found to be close to the bulk amorphous one even for a small fraction of the amorphous phase and almost independent the temperature. We will present the local phonon density of states at different distances from the interfaces. Remarkably, we found that the phonons even at the crystalline part feel the interfaces in a distance of roughly 0.5 nm away from them, and they have density of states similar to the bulk amorphous phase one.

Diameter dependent thermal conductivity of single InAs nanowires for thermoelectric applications

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A large part of used energy is lost as waste heat. Thermoelectric devices form a scalable, solid state solution to recover some of this energy. However, conventional thermoelectric materials suffer from low efficiency and/or high cost. The low efficiency is caused by an interdependency of the parameters in the figure of merit ZT. To overcome this problem nanostructuring has been proposed to independently enhance the thermoelectric properties. To fully exploit these effects a full understanding of the influence of nanostructuring on thermal and electrical behavior is required. Recently considerable theoretical progress has been made, however experimental verification is still lacking. In this work we use InAs nanowires to test some of the predicted effects. We measured the thermal conductivity of wires with diameters ranging from 40 nm to 1.5 µm. We demonstrate a reduction of 80% in thermal conductivity for 40 nm nanowires, opening the way for further design strategies for nanoscaled thermoelectric materials. Furthermore, we investigate the effect of thermal contact in the most common measurement method for nanoscale thermal conductivity.

Phonon scattering enhancement from Si-based nanowires for large thermoelectric figure-of-merits

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Thermoelectric devices have attracted significant research efforts to improve their efficiencies, but thermoelectric properties are strongly correlated, making thermoelectric figure-of-merit (ZT) improvement difficult. One possible approach to avoid such correlation is to suppress phonon transport by scattering phonons at the surface of confined nanowire structures. However, phonon characteristic lengths are often broad in crystalline solids, which makes the confined boundary of nanowires insufficient to minimize heat transport. In this presentation, we will discuss our recent work on the several structures of nanowires employed Ge alloying with Si in order to maximize the depletion of heat-carrying phonons. Silicon germanium ($Si_{1-x}Ge_x$) alloy nanowires are considered one of the most attractive materials for thermoelectric application. Silicon-Germanium homogeneous core-shell alloy nanowires with defected shell and core–shell $Si_{1-x}Ge_x$ nanowires

with controlled structural defects will be discussed for enhancing phonon scattering. Moreover, the nanowire structure for enhancing the electrical properties without increasing the thermal conductivity will be presented.

Complete thermoelectric benchmarking of individual InSb nanowires by combined micro-Raman and transport analysis

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Nanowires are ideal nanostructures for exploring the effects of low-dimensionality and thermal conductivity suppression on thermoelectric behavior. However, it is challenging to accurately measure temperature gradients and heat flow in such systems. Here, using combined spatially-resolved Raman spectroscopy and transport measurements, we are able to determine all the thermoelectric properties of single Se-doped InSb nanowires and to quantify the ZT figure of merit. The measured laser-induced heating in the nanowires and the associated electrical response are well-described by a one-dimensional heat equation. Our results demonstrate that the thermal contact resistances at the source and drain electrodes of the nanowire play a crucial role and cannot be neglected. The measured thermoelectric parameters of InSb nanowires are compared with values obtained by field-effect transistor Seebeck measurements and a good agreement is obtained.

Electron-phonon and phonon-phonon coupling in semiconductors and bismuth: theoretical approaches

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Understanding and predicting the thermoelectric properties of materials, such as the thermoelectric figure of merit ZT, requires reliable theoretical description of both electronic and thermal transport. In this work, we will highlight recent advances in ab intio description of the electron-phonon and phonon-phonon scattering processes in semiconductors and in bismuth, which are crucial ingredients for, respectively, electronic and thermal transport [1,2]. DFT-based calculations of the electron-phonon coupling in semiconductors allowed us to successfully predict the scattering times related to electron-phonon coupling in several semiconductors, as well as in bismuth [1]. We will also show the results of DFT-based calculations coupled with transport equations, in order describe transport properties of semiconductors. Very recently, we have developed a new computational method for the calculation of the electron-phonon coupling in polar materials. This method is based on the interpolation of the electron-phonon matrix elements in Wannier representation. This method allowed us to successfully interpret the dynamics of hot electron relaxation in bulk GaAs, in excellent agreement with time- and angle- resolved photoemission experiment by the group of K. Tanimura (University of Osaka, Japan). The measured, and calculated, electron-phonon scattering times turned out to be surprisingly fast, of the order of a few tens of femtoseconds. In the second part of this talk, we will present our recent results of the ab initio calculations of the thermal transport and phonon-phonon coupling in bismuth. Using recently developed method of the phonon-phonon matrix element calculation, based on density functional perturbation theory, we obtain the lattice thermal conductivity in excellent agreement with experiment and previous theoretical work. Moreover, we discuss the lattice thermal conductivity in the low-temperature regime, and analyze how different phonons

contribute to the lattice thermal conductivity. We show that, surprisingly, the heat is carried by all acoustic phonons over the Brillouin zone, and not only by zone-center phonons.

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Fundamental insight and control into heat transport in silicon-based alloy systems

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Over the last decade, there has been a continued interest in silicon-based thermoelectric (TE) materials because they are cheap and easy to work with and have good modifiable electrical properties. Among them, one promising candidate is silicon-germanium (SiGe) alloy. In order to develop high performance SiGe TE materials, a key issue has been how to further reduce the thermal conductivity (k) of SiGe beyond the so-called alloy limit which is the minimum k of bulk SiGe. While previous attempts have been focused on suppressing thermal conductivity by introducing extrinsic mechanisms of phonon scattering with point-like defects, chemical impurities, and/or grain boundaries, it is important to have a fundamental understanding about intrinsic alloy scattering mechanisms preferentially for efficient design of TE materials. In this presentation, we will describe critical factors determining k of SiGe alloy through a systematic molecular dynamics study of thermal transport with quantum accurate force-field. Furthermore, based on clear understanding about phonon scattering mechanisms of alloy systems, we will discuss the possibility of lowering k below the alloy limit of binary SiGe alloys with utilizing ternary alloying and poly-crystallizing.

Vibrational mode properties in disordered solids

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Due to a lack of short- and long-range order, the vibrational modes in a disordered solid (e.g., alloys, amorphous materials) are not phonons. In this talk, I will discuss how to predict the properties of such vibrational modes, which may be propagating, diffusive, or localized. Both molecular dynamics simulations and lattice dynamics calculations are required. Two case studies will then be presented. First, to assess the virtual crystal approximation, a soft alloy described by a Lennard-Jones potential and a stiff alloy described by the Stillinger-Weber potential are studied. Second, the thermal conductivity accumulation functions for amorphous silica and amorphous silicon are predicted and compared to experimental measurements.

Multiscale modelling of thermoelectrics generators based on graphene nanostructures

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Graphene, which is known to provide very high electrical and thermal conductivities [1][2], might not initially appear as the most natural choice of nanomaterial for energy harvesting through thermoelectricity. However, a giant Seebeck coefficient has been predicted for graphene with periodically patterned electrodes [4] and energy band engineering by appropriate nanostructuring of graphene-based structures makes it possible to tune separately electron and phonon transport properties [3]. In this work, the intrinsic thermoelectric properties of graphene-based nanostructures have been computed within the non-equilibrium Green's function (NEGF) formalism [8]. A fifth nearest-neighbor force-constant model (FCM) [9] and a nearest-neighbor tight-binding Hamiltonian [10] were used to describe phonons and electrons, respectively. Various graphene based nanostructures have been investigated: nanoribbon (GNR) with different

kind of edges [8] and with edge disorder [11], 2D graphene nanomesh (GNM), multilayer of graphene and graphene/BN heterostructures. We show that low thermal conductance, high electronic conductance and enhanced thermopower leading to peak ZT values close to two at room temperature can be achieved by mixing these structures [12]. Theoretical studies on thermoelectricity in nanostructures are usually related only to the calculation of the ZT figure of merit [5][6][7]. We emphasize the need to clarify the extent to which this parameter – derived for dissipative macroscopic structures – reflects the power that can be harvested by ballistic mesoscopic nanostructures. A power analysis of both coolers and generators is conducted by means of multiscale modelling, including thermal contact resistances and electric load resistance, to assess the thermoelectric potential of nanodevices beyond ZT evaluation.

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A multiscale approach for the calculation of transport properties of liquids

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Molecular Dynamics simulations have been performed on Poiseuille-like flows in order to find a linking scheme between atomistic methods and constitutive laws (scaling laws), from nanoscale to macroscale. Simulations have shown that at very small scales there is a considerable effect on transport properties (Sofos et al. 2009). On the other hand computational cost is quite high in order to compute all transport properties. However, we managed to relate the numerical estimates of non-equilibrium molecular dynamics (NEMD) simulations with macroscopic-like relations. The output of this work is that, if the size effect of one of the transport properties is known, then all the others can be estimated from appropriate relations commonly employed for classical fluid mechanics such as the Stokes-Einstein and Sutherland relations (Giannakopoulos et al. 2012). Calculations have been performed for simple fluids (i.e, argon) and results have been found to agree with values given in the literature. The incorporation of new materials on our proposed method could extend the range of applicability so as to contribute on creating nanostructures with specific functionalities, providing design strategies for their synthesis and assembly. This project was implemented under the “ARISTEIA II” Action of the “OPERATIONAL PROGRAMME EDUCATION AND LIFELONG LEARNING” and is co-founded by the European Social Fund (ESF) and National Resources.

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Thermoelectric chip design simulation and EV applications: from quantum mechanics to system dynamics

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This talk will present a multi-scale simulation to study the feasibility, from materials to devices, of thermoelectric air conditioning systems for electric vehicles (EVs). Thermoelectric chips offer the advantages of being solid state, no moving parts, no refrigerants, modular design and easy switch between two modes of either cooling or heating. Nanotech concepts are employed for increasing

the electric conductivity and the Seebeck coefficient, but to reduce the thermal conductivity of those thermoelectric materials. Electron and phonon transport mechanisms are simulated using computational quantum mechanics techniques (CASTEP code based on the density functional theory); while their macroscopic effects are predicted through Boltzmann transport as well as Monte Carlo techniques. System dynamics simulations are carried out based on the Euler-Lagrange framework with passivity control algorithms for the buck/boost converter design. Various nano structure design ideas, including Si-Ge super-lattice, Magnetic Si, organic conducting polymer (PEDOT) nanowires, and transverse effects have been studied and their electron conductivity, electron thermal conductivity, phonon thermal conductivity, Seebeck coefficient, power factor, and figure of merit (ZT) are predicted from the materials aspect. In addition, the coefficient of performance (COP) from the system design aspect has also been studied. A Matlab/Simulink platform will predict the transient performance of the air conditioner (both cooling and heating) in the cabin of an electric vehicle and optimal design from materials to devices of the whole system can be performed.

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