Journées
Plénières

# GdR NAME

**06 - 08**
NOVEMBRE
2024

**IEMN**

*LIVRET*

# *Partenaires et Tutelles*

iemn
Institut d'Electronique, de Microélectronique et de Nanotechnologie
UMR CNRS 8520

Université de Lille

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RENATECH
Le réseau français de nanofabrication

JUNIA Grande école d'ingénieurs

Région Hauts-de-France

# Présentation

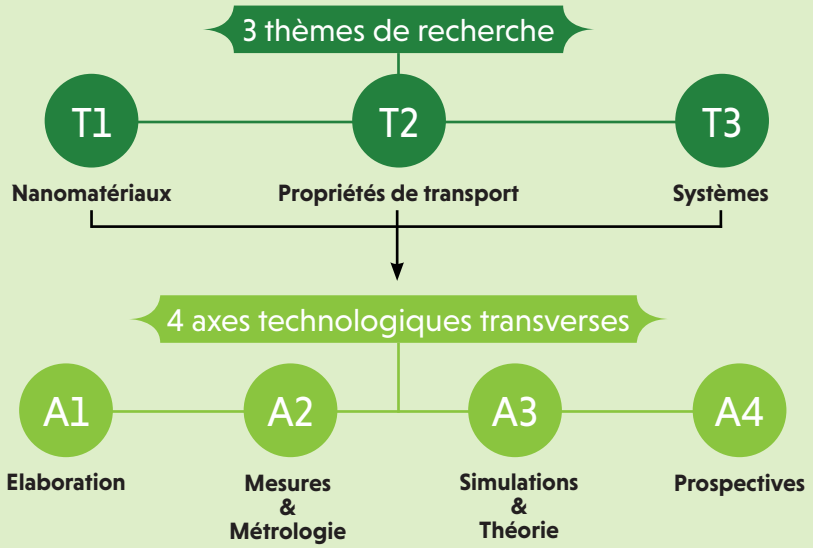
Le Groupe De Recherche « NAnoMaterials for Energy applications » du CNRS vise à élargir les réseaux existants en vue de développer et d'exploiter les spécificités des nanomatériaux pour la récupération, la conversion, le transport, et le stockage de l'Energie.

Créé en janvier 2020, son ambition du GDR «NAME » est de fédérer une communauté scientifique pluridisciplinaire (60 laboratoires avec 550 participants) en provenance de différentes sections (S) et de plusieurs Instituts du CNRS (S10, S8 et S9 de l'INSIS, S3, S4 et S5 de l'INP, S11, S13, S14, S15 et S16 de l'INC).

Cette communauté réunit des scientifiques des domaines de la Physique, de la Chimie, des Sciences des Matériaux et des Sciences de l'Ingénierie et des Systèmes. Elle possède les compétences requises et des savoir-faire uniques à l'état de l'art au niveau national et international en ce qui concerne l'élaboration, la caractérisation et la simulation des nanomatériaux/nanosystèmes pour l'énergie. Plusieurs membres, à l'initiative de cette proposition, étaient déjà impliqués dans des GDR et GDRE soutenus par le CNRS les années antérieures et participent actuellement à des groupements de recherche avec lesquels des ponts pourront être mis en place .

# Thèmes / Axes / Coordination

Afin de proposer et développer des solutions technologiques innovantes pour l'optimisation de la collecte, la conversion et la gestion de petites et moyennes quantités d'énergies disponibles dans la nature et l'environnement, le GDR-NAME est structuré en :






# Comité de Direction

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- **Konstantinos TERMENTZIDIS**, CETHIL, INSA-Lyon

# Programme

## Mercredi 6 Novembre 2024

**8h30 :** Accueil des participants

**8h50 :** Session d'ouverture / Présentation plateformes PCMP ou CMNF

**9h10 :** Invité – **Fabrizio CLERI**

**10h00 :** Pause café

**10h20 :** 1ère session orale avec **Christophe LETHIEN**, **Zacharie WAYSENSON**, **Evgeni STRUGOVSHCHIKOV**, **Jon CANISA DIA** et **Quentin POMPIDOU**

**12h20 :** Déjeuner

**13h50 :** Invité – **Michaël DEPRIESTER**

**14h40 :** Présentation flash posters

**14h50 :** Pause café

**15h10 :** 2ème session orale avec **Pierre-Olivier CHAPUIS**, **François PIQUEMAL**, **Nathaly CHAARAOUI**, **Jordan LETESSIER**, **Markos POULOS** et **Viktor MANDROLKO**

**17h30 :** Table ronde actualités du GDR

**18h30-19h30 :** Exposition posters & Cocktail de bienvenue

## Jeudi 7 Novembre 2024

**09h00 :** Invité – **Alexander PETROV**

**09H50 :** Pause café

**10h10 :** 3ème session orale avec **Olga CUETO**, **Riccardo MESSINA**, **Julien EL HAJJ**, **Isibert NKENFACK** et **Guillaume NATAF**

**12h10 :** Déjeuner

**13h30 :** Présentation de l'écosystème R&D Lillois avec HORIBA (**Lionel LE BIHAN**), l'institut CHEVREUL (**Isabelle DE WAELE**) et CEA Tech (**Olivier DUCLOUX**)

**14h30 :** Visites plateformes PCMP ou CMNF

**16h00 :** Pause café

**16h20 :** Remise du prix de thèse - **Paul DALLA-VALLE**, présentation par **Nicolas CAVASSILAS**



**17h20 :** Table ronde opportunités de financement et montage de projets collaboratifs

**20h00 :** Banquet

## Vendredi 8 Novembre 2024

**08h30 :** Invité – **Masahiro NOMURA**

**09h40 :** Pause café

**10h00 :** 4ème session orale avec **Philippe BASSET**, **Jelena SJAKSTE**, **Marie LESECQ**, **Anass EL FATIMY**, **Shouhang LI** et **Suhao WANG**

**12h20 :** Clôture des journées plénières et Déjeuner

**14h00-16h00 :** Visite plateformes PCMP, CMNF ou institut CHEVREUL

# Conférenciers Invités





## Quantum Heat Machines and Thermodynamics in the 21st Century

• **Fabrizio CLERI** - Université de Lille, IEMN

The thermodynamics of small systems has received a large attention in recent years, also thanks to the development of experiments capable of manipulating single molecules. However, when going at the nanoscale limits, the playground of the quantum regime is entered. The efficiency of heat-to-work conversion in a cyclic heat engine that operates between cold and hot thermal baths with temperature ratio Tc/Th is independent of the specific design, and limited by the universal Carnot theorem.

As opposed to standard heat engines conforming to such a description, diverse models of cyclic engines powered by quantum non-thermal baths have been suggested to function, even at the scale of a single atom, and possibly surpass the Carnot efficiency limit. This brings about several questions for which there is still no clear, rigorously founded answer: Are classical principles still applicable to such devices? Are work and heat properly defined at the quantum scale? Is there a common mechanism for the claims of surpassing of Carnot's bounds? And if there is, does it violate the Second Law of thermodynamics?

# Emerging energy storage miniaturized devices based on thin film technology

**Christophe LETHIEN** - Université de Lille, Réseau RS2E, IUF, IEMN

**Electronic devices and systems are energy-consuming and become ever more miniaturized[1,2]. In that context, the amount of energy required for long-term, sustainable operation is no longer sufficient. A major challenge is to create high-performance but small energy storage sources in a restricted volume. The reached energy density is proportional to the amount of active materials in the electrodes, and two solutions are currently under studied to improve performance, to scale up a technological process while currently investigated fundamental issues such as charge storage mechanisms at electrode/electrolyte interface.**

**One is to maximize the thickness of planar electrodes in lithium-ion micro-batteries[3–5] or micro-supercapacitors[6–9] by depositing several micrometers thick films using magnetron sputtering techniques. Another solution is to develop 3D energy storage microdevices made from a robust 3D scaffold onto which the active materials are conformally deposited[10] using Atomic Layer Deposition[11,12] or pulsed electrodeposition methods[13–15]. Charge storage mechanisms of sputtered metal nitride electrodes for micro-supercapacitors unveiled by in situ, operando and advanced characterization methods will also be presented.**

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# Thermoelectric PEDOT:PSS polymer composites embedded with flower-like quantum dot nanostructures

• **Michaël DEPRIESTER** - Université du Littoral Côte d'Opale – UDSMM

Shivani Shisodia[1], Abdelhak Hadj Sahraoui[1], Dharmendra Pratap Singh[2], Benoit Duponchel[1] and Michael Depriester[1]

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**The rise of low-power communication protocols has created a significant demand for micro energy sources capable of delivering power in the range of hundreds of microwatts [1]. Our surroundings are abundant with diffuse thermal gradients, which can be harnessed to power low-energy systems designed for wireless sensing and data transmission. Thermoelectric (TE) materials offer a solution by converting heat into electricity via the Seebeck effect. This required power can be achieved using standard TE modules with a temperature gradient of just a few degrees under steady-state conditions [2].**

**In this study, EDOT monomers were polymerized in situ with PSS in the presence of titanium dioxide quantum dots decorated graphene oxide (TQDGO) fillers. The thermoelectric properties of the resulting PEDOT:PSS/TQDGO composites, both in bulk and thin film forms, were assessed by varying the filler loading fraction. Electrical conductivity and the Seebeck coefficient were measured, and the Power Factor (PF) was subsequently calculated.**

**A Power Factor (PF) value among the highest reported for conjugated polymers was achieved [3]. Experimental characterizations indicate that thin films outperform their bulk counterparts. This behavior is attributed to the energy filtering effect and the formation of a percolating network that serves as a structural bridge, connecting the PEDOT chains [3,4]. Such nanocomposites hold significant potential for energy applications near room temperature, such as harvesting thermal energy from the human body for remote uses [5].**

References :

[1] M. Haras and T. Skotnicki, Nano Energy, 54, 461-476 (2018).

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## *Local thermal measurements and scanning thermal microscopy*

• **Pierre-Olivier CHAPUIS** - INSA Lyon, CETHIL, CNRS, Université Claude-Bernard Lyon I, France

**Current nanomaterials (wires, 2D, structures surfaces, composites, etc.), including those employed for advanced thermal management, thermoelectricity and optoelectronics, require their thermal properties, such as thermal conductivity, phase change temperature or emissivity, to be accurately determined, in particular at the local scale. In addition, mapping temperature on the surface of active devices with sizes always shrinking can help understanding how hot spots are generated.**

**Optical techniques (thermoreflectance, Raman spectroscopy) or electrical ones (suspended or deposited thermoresistive heaters/sensors or diodes) are options of choice. In this talk, I will especially focus on scanning thermal microscopy, a technique based on atomic force microscopy where tiny thermometers and heaters are embedded on the probe, providing the best prospective spatial resolution.**

Contributors : I will acknowledge the contributions of many colleagues over the years, in particular S. Gomes (CNRS) and W. Zhao (MS student), A.M. Massoud, E. Guen, A. Pic, C. Lucchesi, M. Frausto, J. Sojo, C. Acosta (PhD students), A. Alkurdi (post-doc).

Funding acknowledgements: EU project QuantiHeat and EFINED, and French projects NanoHeat, TIPTOP, ATTSEM, Demo-NFR-TPV, STORE, EF(F)ICACE.

• Alexander Yu Petrov - Hamburg University of Technology - Institute of Optical and Electronic Materials

• Electron photoemission into electrolyte from nanostructured metals

• Although theoretical assumptions on photoemission into electrolyte were formulated more than 90 years ago, the local origin of photo-generated electrons is still a matter of debate. Light absorption can occur in the volume or at the surface of the metal by electron collisions with the boundary. We use nanoporous Au as photoelectrodes and observe the inverse square dependence of emission efficiency on ligament size that confirms the dominant role of surface photoemission.



## *Electron photoemission into electrolyte from nanostructured metals*

• **Alexander PETROV** - Hamburg University of Technology - Institute of Optical and Electronic Materials

**Although theoretical assumptions on photoemission into electrolyte were formulated more than 90 years ago, the local origin of photo-generated electrons is still a matter of debate. Light absorption can occur in the volume or at the surface of the metal by electron collisions with the boundary. We use nanoporous Au as photoelectrodes and observe the inverse square dependence of emission efficiency on ligament size that confirms the dominant role of surface photoemission.**

## *Conditioning systems for triboelectric nanogenerators*

• **Philippe BASSET** - ESYCOM - Marne-la-Vallée

**Triboelectric nanogenerators generate high AC voltages that need to be rectified and converted to a low DC value in order to power typical electronic devices. The criteria for defining the best conditioning circuit and power management architecture depend on many parameters, such as the maximum voltage supported by the system, the value of the final DC voltage, the number of actuations before the harvested electrical energy must be supplied, the built-in voltage and capacitance variation of the TENG, or the losses of key components such as diodes or switches.**

**Two main families of conditioning circuits can be used to convert output voltage from AC to DC, stable and unstable charge pumps [1], and among them, several choices are possible [2]. In this presentation, we will introduce the most common circuits for conditioning electrostatic generators such as TENGS and discuss some criteria for their optimization [3] [4].**

References :

1] A. Ghaffarinejad et al., « A conditioning circuit with exponential enhancement of output energy for triboelectric nanogenerator », Nano Energy, vol. 51, p. 173-184, sept. 2018

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## *Simulation des mécanismes de changement de phase dans des mémoires PCM avec la méthode multi-champ de phase couplée à un solveur électro-thermique.*

• **Olga CUETO** - CEA-Leti - Grenoble

**Les mémoires à changement de phase (PCM) stockent l'information binaire dans la phase d'un matériau qui peut être soit cristallin, soit amorphe. Ces deux états ayant des résistivités électriques différentes, il est possible de les distinguer et de lire l'information stockée. Pour écrire dans la mémoire, le matériau est chauffé localement par effet Joule avec un courant de forte intensité. L'alliage GST225 est largement utilisé pour les PCM car il cristallise rapidement et sans changement de composition. Cependant, il présente une mauvaise rétention de l'information au-delà de 100°C, ce qui le rend incompatible avec certaines applications comme l'automobile. Pour ces applications, STMicroelectronics (STM) utilise un alliage modifié, enrichi en Ge (GGST) stable à haute température.**

**Nous présenterons dans cet exposé le travail réalisé dans le cadre de deux thèses CIFRE avec STM réalisées au LETI sous la direction de Mathis Plapp chercheur au Laboratoire de Physique de la Matière Condensée de l'Ecole Polytechnique. Nous avons développé un outil de simulation reposant sur la méthode champ de phase pour simuler la cristallisation complexe de l'alliage GGST et nous avons couplée cette méthode à un solveur électrothermique qui lui-même prend en compte les phases du GGST. Par ce couplage, nous avons un simulateur capable de rendre compte de la production de chaleur par la cristallisation et par effet Joule , ainsi que de la propagation dans les différents matériaux constituant la mémoire. Les conductivités électrique et thermique du GGST utilisées dans le solveur électrothermique dépendent de la phase et par conséquent les évolutions de la microstructure dans le GGST influencent le comportement électrothermique du matériau.**

## *Planar-type nanostructured Si thermoelectric energy harvester*

• **Masahiro NOMURA** – Institute of Industrial Science, the University of Tokyo

**We demonstrate Si thermoelectric generator (TEG) with output power exceeding 100μW for energy harvesting application. We designed and fabricated the planar-type Si TEGs using nanostructured Si thin film and three-dimensional micro heat guiding structures. The phononic crystal (PnC) nanostructure reduces the phonon mean free path by surface scattering and increase the temperature gradient in Si thin film while keeping electrical resistance low. The normalized power density of TEG reached 1.3 μWcm-2K-2 which is the highest ever reported for planar-type Si thin film TEGs.**



## *Modélisation et conception d'un système de craquage solaire de l'eau basé sur des hétérojonctions de van der Walls*

• **Paul DALLA-VALLE** - IM2NP

# Abstracts

**• Suhao WANG (p20)**

*Remarkable Enhancement of Thermoelectric Properties of Conjugated Polymers by Suppressing Dopant-Induced Disorder*

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**• Viktor MANDRILKO (p21)**

*Understanding Heat Transport across Functionalized Silica-Water Interface: Insights from Molecular Dynamics Simulations*

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**• Evgeni STRUGOVSHCHIKOV (p22)**

*Atomistic Insights into Hydrazine Hydrate Oxidation Reaction on Nickel Catalysts: The Role of Co-Adsorbed Species in Bond Breaking Selectivity*

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**• Markos POULOS (p23)**

*Temperature-Dependent Phonon Energies and Lifetimes in Single and Few-Layer Graphene using Molecular Dynamics*

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**• Anass EL FATIMY (p26)**

*Boosting Organic Solar Cell Performance via Metalloporphyrin Encapsulation: Investigating Charge Transfer and Fermi Level Shifts in Single-Walled Carbon Nanotubes*

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**• Riccardo MESSINA (p27)**

*Focusing of heat flux radiated by magneto-optical nanoemitters in the presence of a magnetic-field*

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**• Julien EL HAJJ (p28)**

*Enhanced thermal conductance at interfaces between gold and amorphous silicon and between gold and amorphous silica*

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**• Jordan LETESSIER (p29)**

*Temperature measurement in semitransparent media using photothermal heterodyne imaging*

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**• Isibert NKENFACK (p30)**

*Study and modelling phonon transport in SiGe and InGaAs alloys*

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**• Guillaume NATAF (p31)**

*Domain-wall induced decrease in thermal conductivity with increasing grain size in ferroelectric ceramics*

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**• Jelena SJAKSTE (p32)**

*Occurence of the collective Ziman Limit of heat transport in cubic semiconductors : Scattering channels and size effects*

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**• Zacharie WAYSENSON (p33)**

*Simulations of electrochemical systems with flexible electrode models*

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**• Nathaly CHAARAOUI (p34)**

*Approche inverse pour l'analyse thermique de nanomatériaux via microscopie à sonde locale*

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**• Quentin POMPIDOU (p35)**

*Thermal boundary conductances measurements of metal/semiconductor junction by means of photothermal radiometry*

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**• Jon CANOSA DIAZ (p36)**

*Silicon Based Suspended Thermometry Device Fabrication for Study of Phonon Transport Phenomena in the Ballistic and Coherent Regimes*

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**• Marie LESECQ (p37)**

*Thermal properties of 3C-SiC thin layer used to improve heat dissipation in GaN based HEMTs*

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**• Shouhang LI (p38)**

*Lattice Thermal Conductivity of Single Polymer Chains from First-principles Including Quantum and Anharmonic Effects*

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# Remarkable Enhancement of Thermoelectric Properties of Conjugated Polymers by Suppressing Dopant-Induced Disorder

Suhao Wang [1], Stephane Longuemart [2], and Henning Sirringhaus [3]

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**3** The Cavendish Laboratory – JJ Thomson Avenue, Cambridge, CB3 0HE, United Kingdom

**Doping is an enabler in both conventional organic electronics such as organic solar cells and organic field-effect transistors and emerging electronic devices such as organic thermoelectrics.(1)**

**However, a long-lasting challenge, that has been limiting the achievable performance of various electronic devices, is the trade-off between achieving a high doping level and minimizing dopant-induced structural disorder.(2) Research on minimizing structural disorder and maximizing charge carrier mobility in the doped state is still rarely reported.**

**Here, we show that by ion-exchange doping polythiophene-based P((3HT)1-x-stat-(T)x) (x = 0 (P1), 0.12 (P2), 0.24 (P3), and 0.36 (P4)), remarkably high electrical conductivity of > 400 S/cm and power factor of > 16 μW/mK2 were achieved for the random copolymer P3, ranking it the highest ever reported for unaligned P3HT-based films, significantly higher than that of P1(P3HT).(3)**

**Although P1 and P3 exhibit comparable hole mobilities in the pristine state, after doping, Hall effect measurements indicate that P3 exhibits a significantly large Hall mobility. GIWAXS measurement determined that the in-plane π-π stacking distance of doped P3 is much shorter than that of doped P1. Moreover, the doped film exhibits satisfying ambient stability, (3) which can be explained by the recent investigation on phaseselective doping of conjugated polymers.(4)**

**This work offers an effective strategy to realize fast charge transport in highly doped conjugated polymers and highlights the importance of overcoming dopant-induced disorder to achieve next-generation efficient organic electronics.**

References :

(1) S. Wang*, et al., Prog. Polym. Sci., 2022, 129, 101548.

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# Understanding Heat Transport across Functionalized Silica-Water Interface: Insights from Molecular Dynamics Simulations

Viktor Mandrolko[1], David Lacroix[1], and Mykola Isaiev[2]

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**2** Laboratoire d'Energies et Mécanique Théorique et Appliquée – Université de Lorraine, Centre National de la Recherche Scientifique : UMR7563 / URA875, France

**Thermal transport across solid/liquid interfaces is critical in many applications, influencing heat exchange efficiency in various systems. One of the ways for the tuning of the interfacial properties is surface functionalisation.**

**The properties of the silica surface, a widely used material in micro/nanofluidics, can be significantly altered through functionalisation with groups such as hydroxyl (-OH) and methyl (-CH3), impacting both adhesion and thermal resistance. In this study, we investigate the effect of varying concentrations of hydroxyl and methyl groups on the thermal transport across silica-water interfaces using molecular dynamics simulations.**

**The wetting behaviour and interfacial thermal resistance (ITR) were analysed for different surface functionalization levels, revealing a strong correlation between surface functionalisation and thermal resistance and wetting characteristics.**

# *Atomistic Insights into Hydrazine Hydrate Oxidation Reaction on Nickel Catalysts: The Role of Co-Adsorbed Species in Bond Breaking Selectivity*

Evgenii Strugovshchikov[1], Evgeniia Vorms[2], Antoine Bonnefont[3], Marian Chatenet[3], Alexandr Oshchepkov[2], Olivier Lottin[1,4], Elena Savinova[2], and Mykola Isaiev[1]

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**Hydrazine (N2H4) is a promising carbon-free fuel for electrochemical energy generation due to its high hydrogen content and environmentally friendly byproducts. Nickel (Ni) nanoparticles are effective catalysts for the hydrazine hydrate oxidation reaction (HHOR), but the complete atomistic mechanism remains unclear.**

**Using ab initio methods, we investigate the role of co-adsorbed species, including hydrogen (Hads), hydroxide (OHads) and water (H2Oads), on HHOR kinetics. Our findings show that OHads significantly promote N-H bond cleavage, reducing surface poisoning and enhancing reaction selectivity on Ni surfaces, which agrees with the experimental results.**



# *Temperature-Dependent Phonon Energies and Lifetimes in Single and Few-Layer Graphene using Molecular Dynamics*

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**In this work, we investigate the phonon properties of multilayer graphene (1-5 layers) and bulk graphite using Molecular Dynamics (MD) simulations with the k-space Autocorrelation Sequence (k-VACS) method. From the MD-derived atomic trajectories, we compute the Velocity Autocorrelation Function and use Fourier Transform to obtain the Phonon Spectral energy Density (PSD).**

**This allows us to extract temperature-dependence of phonon energies and lifetimes, as well as the phonon Densities of States (DOS) across a temperature range of 80-1000 K. We examine how the number of graphene layers affects the phonon energies and lifetimes, focusing particularly on -point phonons and comparing the effects of different interlayer potentials (Kolmogorov-Crespi and Lennard-Jones).**

**Our results show that while the number of layers has minimal impact on intralayer (ZO, G) phonon energies, it significantly influences phonon lifetimes, as well as the energies of the interlayer modes. Notably, the lifetime of the Raman-active G phonon increases with the number of layers, regardless of the interlayer potential used, which is directly related to the coupling strength of the interlayer interaction. This work presents several novel findings on phonon properties of multi-layered graphene, notably the temperature dependence of interlayer phonon modes and the effect of layer number on G phonon lifetimes.**


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# *Boosting Organic Solar Cell Performance via Metalloporphyrin Encapsulation: Investigating Charge Transfer and Fermi Level Shifts in Single-Walled Carbon Nanotubes*

Anass El Fatimy[1], Mourad Boutahir[1], Konstantinos Termentzidis[2], and AbdelaliRahmani[1]

**1** LEM2A – Morocco

**2** CEHTIL – CNRS – France

This research investigates the integration of metalloporphyrin molecules within semiconducting single-walled carbon nanotubes (SWCNTs) to create an active layer for solar cells. By employing density functional theory, we examine the optoelectronic characteristics of metalloporphyrin molecules encapsulated inside SWCNTs. Our findings suggest that the structural stability arises from electrical charge transfer between the nanotube and the metalloporphyrin.

The metal atoms were carefully chosen for their notable influence on the hybrid's electronic properties, resulting in enhanced light absorption, better charge separation, and improved power conversion efficiency in solar cells. A shift in the nanotube's Fermi level after encapsulation points to a relationship between charge transfer and metalloporphyrin-nanotube interaction.

These results suggest that the encapsulated systems, forming type II heterojunctions, could serve as efficient charge carriers and light absorbers in organic solar cells featuring filled SWCNTs. This study presents a promising step toward the development of high-performance organic solar cells utilizing these hybrid structures.



# *Focusing of heat flux radiated by magneto-optical nanoemitters in the presence of a magnetic-field*

Louis Rihouey[1], Philippe Ben-Abdallah[1] and Riccardo Messina[1]

**1** Laboratoire Charles Fabry – Université Paris-Saclay,Sorbonne Universités, Institut d'Optique Graduate School, CNRS – France

We introduce a theoretical framework to describe the heat flux radiated in the near-field regime by a set of magneto-optical thermal nanoemitters close to a substrate in the presence of an external magnetic field. Then, we investigate the particular case of a single emitter and we demonstrate that the external field can induce both an amplification of the heat exchanged between emitter and substrate and a focusing of the Poynting field at the substrate interface at deep sub-wavelength scale. These effects open up promising perspectives for the development of heat-assisted magnetic-recording technology.

## *Enhanced thermal conductance at interfaces between gold and amorphous silicon and between gold and amorphous silica*

Julien El Hajj[1]

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**Gold core-shell nanoparticles have shown remarkable potential in a variety of biomedical applications. In this study, we employ non-equilibrium molecular dynamics simulations to investigate the interfacial thermal conductance of gold and two different materials, silicon and silica, in both their crystalline and amorphous structures. The results show that gold and amorphous structures have significantly higher interfacial thermal conductance than crystalline structures.**

**We explain this increase by investigating the modal contributions of elastic and inelastic tran mission to heat conduction. We demonstrate that all vibrational modes contributing to inter-facial heat transfer are delocalized and use the Ioffe-Regel criterion to distinguish between propagating and non-propagating modes.**



## *Temperature measurement in semitransparent media using photothermal heterodyne imaging*

Jordan Letessier[1], Jérémie Maire[1], Stéphane Chevalier[1,2] and Abel Netter[1]

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**2** Ecole Nationale Supérieure d'Arts et Métiers (ENSAM) - Bordeaux – Ecole Nationale Supérieure d'Arts et Métiers (ENSAM) - Bordeaux – France

**In this study, we use photothermal heterodyne imaging to measure the thermo-optical transmission coefficient of three materials : Borofloat glass, PDMS, and pure water. Utilizing this coefficient, we further map the temperature fields in several samples of varying thicknesses with a resolution of 26 µm.. A pseudo 1D thermal model is employed to validate our measurements, demonstrating the accuracy and reliability of the proposed approach for a wide range of materials. Additionally, this technique holds potential for applications in microfluidics, where precise thermal mapping at the microscale is crucial.**

## *Study and modelling phonon transport in SiGe and InGaAs alloys; application to thermal conductivity calculations*

Isibert Nkenfack[1]

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**Understanding heat transport phenomena and controlling thermal properties in semiconductor alloys are crucial for improving the efficiency of advanced electronic devices and energy harvesting through thermoelectric materials. In this context, we studied the thermal conductivity of SiGe and InGaAs alloys. Our work is based on model development and various numerical simulation methods with experimental data available in the literature.**



## *Domain-wall induced decrease in thermal conductivity with increasing grain size in ferroelectric ceramics*

Rachid Belrhiti Nejjar[1], Fabien Giovannelli[2], Jan Schultheiß[3], Manuel Zahn[3], Dennis Meier[3], and Guillaume Nataf[1]

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**2** Laboratoire GREMAN, CNRS, Université de Tours, UMR 7347, 41029 Blois, France – GREMAN UMR 7347 – France

**3** Norwegian University of Science and Technology – Norway

**Smaller grains lead to lower thermal conductivities. This correlation proposed theoretically by Kittel in 1949 for glasses has been then demonstrated experimentally in all solids, from graphene to metals to oxides. Here, it is found that polycrystalline ceramics of the improper ferroelectric ErMnO3 exhibit the opposite behavior: the thermal conductivity increasesfrom 3.2 to 4.2 W m-1 K-1 with decreasing grain sizes from 8.4 to 1.2 µm, in the full temperature range studied (- 100oC to + 100oC).**

# Occurence of the collective Ziman Limit of heat transport in cubic semiconductors : Scattering channels and size effects

Jelena Sjakste, Maksim Markov, Raja Sen, Giorgia Fugallo, Lorenzo Paulatto and Nathalie Vast

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**The study of the heat transport regimes in bulk and low dimensional materials in general, and of the phonon hydrodynamics in particular, currently attracts a renewed interest. While it was observed in graphene, graphite, black phosphorus and SrTiO3, the collective limit of heat transport, referred to as hydrodynamic regime, or Ziman limit, was observed only in relatively few "common" 3D materials, such as Bi, solid helium and NaF at cryogenic temperatures.**

**In materials such as natural Si and Ge, the dominance of resistive processes, and in particular scattering by isotopes, prevents the occurrence of the collective limit. At the same time, methods based on the density functional perturbation theory and on the Boltzmann transport equation (1,2) were shown to accurately predict the conditions of the occurrence of the collective limit of heat transport in many materials (2,3). In this work we have studied the conditions of the occurrence of the collective Ziman limit of heat transport in cubic semiconductors, such as silicon, germanium, AlAs and AlP, as a function of isotope composition and at temperatures below 50 ¯K (4).**

**We show that while in natural and enriched silicon and germanium the collective heat tran port limit is impossible to reach due to strong isotopic scattering, in hyper-enriched silicon and germanium, as well as in materials with one single stable isotope like AlAs and AlP, at low temperatures, normal scattering plays an important role, making the observation of the collective heat transport possible.**

**We further discuss the effects of sample sizes, and analyse our results for cubic materials by comparing them to bulk bismuth, in which second sound has been detected at cryogenic temperatures. We find that collective heat transport in cubic semiconductors studied in this work is expected to occur at temperatures between 10 and 20 K (4).**

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# Simulations of electrochemical systems with flexible electrode models

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**Electrochemical energy storage devices, such as batteries and supercapacitors, play an important role in the ongoing energy transition. To further optimize their performance, a deep understanding of these devices is crucial. Atomistic simulations provide a unique opportunity to model these systems at the atomic scale under various operating conditions. Recent advancements have enabled explicit modeling of processes like supercapacitor charging (S. Bi and M. Salanne, ACS Nano (2022)).**

**However, current approaches often simplify electrode models, neglecting their mechanical dynamics, which may impact results, especially when coupled with ion dynamics. It seems interesting to integrate Machine Learning Potentials, which are particularly effective for short-range interactions, with long-range physical models for describing electrostatic interactions. Testing the influence of the electrodes dynamics with several potentials such as AIREBO (Stuart, Steven J. et al., J. Chem. Phys. 112 (2000) ) or the Atomic Cluster Expansion potential (Ralf Drautz, Phys. Rev. B (2019)) demonstrated promising results, revealing discrepancies in key supercapacitor properties across models used for electrode dynamics.**

**Recent simulations showcased a notable decrease in charging time and increase in capacitance for flexible electrodes models, motivating further exploration into the influence of electrode dynamics on supercapacitor performance. Drawing inspiration from studies on carbon electrode morphology (EH Lahrar et al., J. Chem. Phys. 155, 184703 (2021)), our study is focused on a system composed of graphitic nanoporous electrodes in contact with ionic liquid electrolyte.**

**Using recent advancements in the Performant Atomic Cluster Expansion model (Minaam Qamar et al., J. Chem. Theory Comput. (2023)), the objective is to understand the intricate relationship between electrode dynamics, capacitance, and ion adsorption mechanisms under diverse potential differences. This research not only advances fundamental understanding but also holds promise for optimizing future energy storage device design and performance.**

# *Approche inverse pour l'analyse thermique de nanomatériaux via microscopie à sonde locale*

Nathaly Chaaraoui, Nathalie Trannoy, and Thierry Duvaut

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Les nanotechnologies exigent des méthodes spécifiques de caractérisation pour les nanosystèmes et les nanomatériaux. Une compréhension avancée du transfert de chaleur à l'échelle nanométrique et des propriétés thermiques des matériaux nanostructurés est cruciale pour l'innovation de nouveaux matériaux. Les propriétés thermiques des couches minces ont été minutieusement explorées pour divers matériaux, et la microscopie thermique à sonde locale (SThM), basée sur la microscopie à force atomique (AFM), s'avère être un outil essentiel pour étudier localement le comportement de ces matériaux et les mécanismes de transfert de chaleur à l'échelle micro/nanométrique. Ce projet vise à évaluer les propriétés thermiques locales de matériaux nanostructurés.

A cette fin, deux échantillons à la nanostructure enterrée ont été spécialement conçus. Le premier présente une marche triangulaire subsurfacique en SiO2 déposée sur un substrat en silicium, recouverte de SiO2 CVD poli. L'interface SiO2/Si est linéaire, avec une épaisseur variant entre 400 et 2150 nm. Le second est composé de trois marches de SiO2 d'une épaisseur de 260 nm recouvertes d'une couche de SiO2, déposées sur un substrat de silicium. Ces deux géométries différentes visent à étudier la réponse de la microsonde en terme de structuration interne de l'échantillon et ainsi évaluer la conductivité thermique locale du SiO2.

Pour obtenir des informations thermiques sur les matériaux nanostructurés, le microscope thermique (SThM) doit être équipé d'un capteur thermique, permettant l'acquisition simultanée d'images topographiques et thermiques. Une sonde thermosensible micrométrique en Wollaston a été sélectionnée à cette fin. Pour interpréter les résultats expérimentaux de SThM, un modèle de transfert de chaleur par la méthode des éléments finis (FEM) du système sonde-échantillon a été développé pour (a) étudier l'impact de la structure de l'échantillon sur le signal thermique de la sonde, et (b) caractériser la conductivité thermique locale.

A partir du modèle numérique, une technique inverse a été mise en oeuvre en utilisant l'algorithme Levenberg-Marquardt combinant deux méthodes inverses : la méthode de Gauss-Newton et la méthode de descente conjuguée, pour évaluer la conductivité thermique locale à partir des puissances dissipées par la sonde. Cela a permis de déduire celle de la couche de SiO2 d'épaisseur variable sur le substrat de silicium. Le modèle numérique, basé sur le couplage électrothermique de la sonde/échantillon, évalue le flux dissipé par l'élément thermorésistif et vers l'échantillon. La comparaison entre la simulation et les mesures expérimentales démontre que le modèle reproduit les profils thermiques expérimentaux pour l'échantillon avec une épaisseur variable de SiO2.

Il est à noter que la conception de l'échantillon assure une résistance thermique de contact constante à chaque point de mesure. Nos résultats montrent une diminution de la conductivité thermique avec l'épaisseur de la couche de SiO2. Ces constations ont été confirmées par une analyse supplémentaire effectuée sur une nanostructure présentant une configuration distincte. Il en résulte que le matériau, au-delà de 1400 nm, adopte un comportement similaire à celui d'un échantillon massif, tandis qu'en dessous de cette valeur, la conductivité thermique que nous avons pu quantifier dépend de l'épaisseur du matériau.



# *Thermal boundary conductances measurements of metal/semiconductor junction by means of photothermal radiometry*

Quentin Pompidou and Nicolas Horny

ITheMM – Université de Reims Champagne Ardenne (URCA) – France

As power consumption rises and electronic component's size decrease, the challenge of dissipating heat remains a challenge for modern technologies. The main issue lies in the thermal transport at nanoscale interfaces. This study aims to enhance our understanding of heat transfer at metal/semiconductor junctions, focusing on Thermal Boundary Conductance (TBC) and its influences with electrical properties.

# *Silicon Based Suspended Thermometry Device Fabrication for Study of Phonon Transport Phenomena in the Ballistic and Coherent Regimes*

Jon Canosa Diaz[1], Hafsa Ikzibane[1], Boris Brisuda[2], Carlos Polanco[3], Marc Dewite[4], Natalio Mingo[3], Olivier Bourgeois[2], Emmanuel Dubois[1], and Jean-Francois Robillard[1]

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**3** Laboratoire d'Innovation pour les Technologies des Energies Nouvelles et les nanomatériaux – CEA-LITEN – France

**4** Institut d'électronique, de microélectronique et de nanotechnologie (IEMN) – CNRS : UMR8520, Institut supérieur de l'électronique et du numérique (ISEN), Université Lille I - Sciences et technologies, Université de Valenciennes et du Hainaut-Cambrésis – France

**This works addresses the current experimental gap in thermal transport regimes and phonon transport at low temperatures and small scales. We have fabricated a SOI based suspended thermal sensor platform functional from room temperature down to 55 mK. The device will be used for the study of phonon transport across several Si-based samples like phononic crystals, metamaterials and nanowires.**



# *Thermal properties of 3C-SiC thin layer used to improve heat dissipation in GaN based HEMTs*

Marie Lesecq, Pierre-Yves Cresson, Ghizlane Boussatour and Zahia Bougrioua

IEMN-Institut d'Electronique de Microélectronique et de Nanotechnologie, F-59000, Lille – Université de Lille - Sciences et Technologies, IEMN-CNRS 8520, Université des Sciences et Technologies

**This work reports on the thermal conductivity measurements of 3C-SiC thin layers using the 3ω electro-thermal method. The 3C-SiC layer is of great interest if used as an inter-layer for AlGaN/GaN HEMT grown on silicon substrate to enhance heat dissipation. An analysis of the initial thermal measurement results highlights the limitations of 3ω method and led us to move towards a new approach with suspended 3C-SiC layer to reach more accurate results on thermal conductivity.**

## Lattice Thermal Conductivity of Single Polymer Chains from First-principles Including Quantum and Anharmonic Effects

Shouhang Li
Université Paris-Saclay – university – France

**Molecular crystals possess numerous advantages, and understanding the upper limit of their lattice thermal conductivity is crucial. However, the classical molecular dynamics simulation and standard first-principles calculation fail to predict the lattice thermal conductivity of single polymer chains. In this work, we applied the stochastic self-consistent harmonic approximation to obtain the physically meaningful vibrational properties of single polymer chains. It is found that quantum and anharmonic effects have significant influences on their lattice thermal conductivities.**



# Posters

## Silicon Materials Mid-Infrared Direct Spectral Emissivity Measurement at Intermediate

Elissa Akiki, Armande Herve, Georges Hamaoui, Marty Frederic, Tarik Bourouina, Philippe Basset and Elyes Nefzaoui
ESYCOM, Université Gustave Eiffel, CNRS UMR 9007, F-77454 Marne-la-Vallée, France – ESIEE

**This study introduces a test bench developed for the direct measurement of material emissivity, which is crucial for enhancing the efficiency of systems involving thermal radiation control or conversion such as radiative cooling, solar cells, thermophotovoltaics (TPV) and infrared (IR) photodetectors. Currently under development, this test bench is designed to operate at intermediate temperature ranges from 300oC to 600oC. It is engineered to enable direct and spectral measurements, thereby improving the understanding of emissivity's, spectral, and temperature dependences.**

**We also report on results obtained for silicon, a material widely used for thermal radiation control and conversion devices, at different doping levels and different temperatures. Obtained results can be useful to assess the suitability of these materials and related meta-materials for different applications where emissivity at intermediate temperatures plays a major role.**

## *Nanoscale thermal transport in self-assembled ordered nanocrystal solids*

Matias Feldman, Charles Vernier ,Rahul Nag ,Sebastien Royer ,Hervé Cruguel ,Emmanuelle Lacaze , Emmanuel Lhuillier ,Danièle Fournier ,Florian Schulz ,Cyrille Hamon , Hervé Portalès and James K. Utterback

Institut des Nanosciences de Paris – Sorbonne Universités, UPMC, CNRS – France

Nanocrystal based solids are a promising class of materials whose emergent properties are highly tunable as a function of constituent shape, size, material composition and surfacecapping ligands. They are of particular interest for the development of plasmonic, optoelectronic and thermoelectric devices. Understanding and controlling heat flow in these materials is one of the last steps preventing their mass adoption as heating due to optical excitation or current leads to performance degradation, instability and unwanted chemical activity. I will present recent results on the thermal properties of supercrystals of gold nanospheres, nanorods and nano-bipyramids.

Thanks to correlative SEM and spatio-temporally resolved thermoreflectance we were able to access sub-micron structural and nanosecond dynamical thermal information. We demonstrated that heat flow predominantly follows the orientation of the elongated nanoparticles and does so even in curved assemblies. In ordered superlattices, heat transport is anisotropic flowing faster along the particles' long axis.

Our measurements together with finite element simulations and effective medium modelling show that this anisotropy can be finely tuned through the nanoparticles aspect ratio, shape and packing. Leveraging this anisotropy opens the way to enhanced thermal dissipation and thermal routing directly using the device's active material.



## *ZnO nanopillars and liquid crystals for hybrid solar cells*

Bator Khol

UCCS Equipe Couches Minces Nanomatériaux – Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France

With the ever-increasing global population and the resulting energy demand, it is crucial to develop renewable energy sources to replace fossil energies. In this context, our research focuses on designing a simple and cost-effective alternative to current silicon-based solar cells, which also have relatively polluting chemistry (1). This work aims to develop solar cells by exploiting P/N heterojunctions based on semiconducting liquid crystals materials ((1) benzothieno(3,2-b)(1) benzothiophene: (Ph-BTBT-10)) and zinc oxide (ZnO) nano-pillars (2,3).

In this work, we present the synthesis of ZnO nanopillars with a nanometric controlled diam ter by electrodeposition on different substrates (glass with transparent conducting oxides and Platinum layer deposited on Silicon substrate), followed by the impregnation of Ph-BTBT-10 liquid crystal molecules on the ZnO nano-pillars. The electrodeposition method offers an optimal architecture to maximize the surface of interaction between ZnO nanopillars and the Ph-BTBT-10 molecules (4).

The structure of these nanowires is characterized by X-ray diffraction and scanning electron microscopy. These analyses demonstrate the specific growth of nano-pillars with a strong anisotropy which can described by the c-axis perpendicular to the substrate. In addition, the electrical behavior of these samples was analyzed by a photo-electrochemical setup equipped with different light diodes, Mott-Schottky curves). And finally, the current-voltage characteristic of our solar cell was measured under the light provided from a solar simulator.

# *Investigation of thermoelectric properties in Silicon Nanostructures using particle Monte Carlo Simulation*

Mohamad Ghanem[1], Jerome Saint-Martin[1,2], and Philippe Dollfus[1]

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**2** Ecole Normale Supérieure Paris-Saclay – Université Paris Sud, Université Paris Saclay – France

**A silicon based nanofilm is examined by using self-consistent electron-phonon transport model. An ensemble Monte Carlo solver for electrons is coupled with a phonon bath that can have a non-uniform temperature. In this simulator, the electron-phonon scattering rates depend on the local temperature and the boundary conditions are also temperature dependent. Using this simulation tool, the thermoelectric properties can be studied, at the microscopic level, in doped silicon nanostructures of different sizes and with different types of interfaces. In the present work, the diffusive Seebeck coefficient of silicon-based nanofilms is investigated under the influence of the temperature, temperature gradient, device size, and carrier concentration.**



## Notes

# Gala à la péniche « L'Aristote»

## 02 ISOCRATE

4 points boissons par personne*

1ère partie :
- Mini tartare de boeuf sur toast
- Tenders de poulet et wings de choux-fleur
- Sablés au parmesan et sa mousse de chèvre

2nde partie :
- Frites maison au couteau
- Bavette d'Aloyau cuisson au four à bois (70gr p. pers)

3ème partie :
- Camembert au four à bois

4ème partie :
- Gâteau au choix**, Mousse au chocolat, Tiramisu spéculoos ou Panna cotta au coulis de fruits

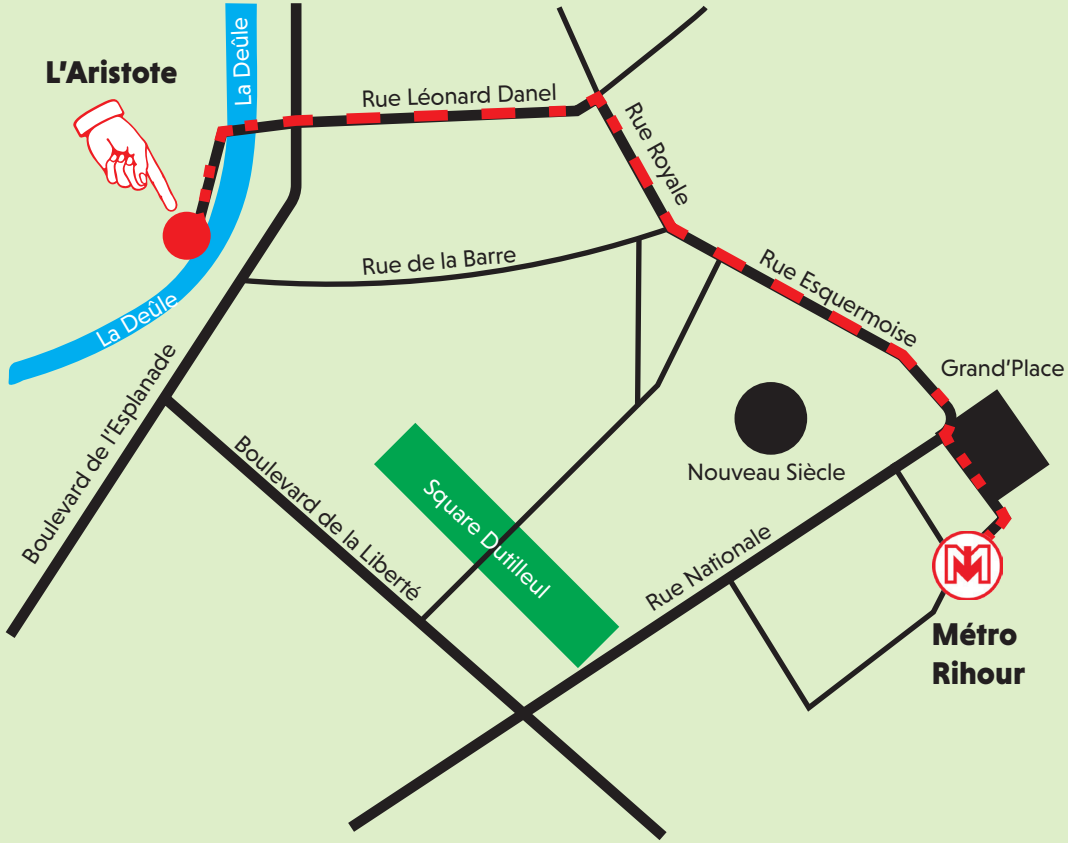
* 1 point : 1 verre de vin 12cl, bière 33cl, cocktail sans alcool ou soft
2 points : une coupe de champagne ou un cocktail



# Accès

Prendre le métro 4 Cantons jusqu à l'arrêt Rihour (15 minutes)

Suivre l'itinéraire indiqué ci-dessous (15 minutes à pied)



# Numéros si besoin, renseignement ou problème :

*« La science n'a pas de patrie, parce que le savoir est le patrimoine de l'humanité, le flambeau qui éclaire le monde. »*

Louis PASTEUR

Plus d'infos