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NanoThermique, mesures

Molecular Dynamics Simulations of the Influence of Domain Walls on the Thermal Conductivity in Barium Titanate BaTiO3

Ilyass Aabouch * [1], Guillaume F. Nataf *

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In order to build intelligent thermal devices and low-cost supercomputers, controlling heat flow through materials has become a very attractive and reliable approach (1). In our study, we investigated the influence of domain walls on the thermal conductivity in the ferroelectric material BaTiO3 using Nonequilibrium Molecular Dynamics simulations within the LAMMPS framework. We study how different parameters could influence the thermal conductivity in BaTiO3 such as the number of domain walls

(1): C. Wang, L. Hua, H. Yan, B. Li, Y. Tu, and R. Wang, "A thermal management strategy for electronic devices based on moisture sorption–desorption processes," Joule 4, 435–447 (2020).

Keywords: Thermal Conductivity, ferroelectric

*Speaker

Spatiotemporal Microscopy of Thermal Dynamics from Nanomaterials to Phase-Change Materials

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The functionalities of photoactive materials ranging from optoelectronics, plasmonics, catalysis and phase-switching applications require not only control over the photoexcited charges but also heat generation, transport and dissipation. Controlling nanoscale thermal transport is fundamental to virtually all such applications, as they either inherently generate heat as a byproduct or deliberately harness it for operation. While pump–probe spectroscopy signals are typically attributed to electronic energy carriers (i.e., electrons, holes, excitons), there is increasing recognition that laser induced heating can also lead to transient spectral signals in semiconductor films. On one hand there is a need to better understand the contributions of heating to pump–probe measurements for accurate assignments, and at the same time this presents opportunities to investigate microscopic thermal transport and dissipation. Recent advances in thermoreflectance have enabled critical temporal and spatial thermophysical characterization to probe the mechanistic impact of nanoscale structuring on heat propagation. In this presentation I will describe how pump–probe optical measurements and modeling of thermal transport provide access to nanosecond dynamical information with local, sub-micron specificity. I will highlight examples including metallic nanocrystal superlattices, semiconductor nanocrystal films, and insulator-to-metal phase transition thin films. We will touch on questions including: How do heterogeneous environments and interfaces impact microscopic energy transport? How can we access information about energy carriers that traditionally do not have clear spectroscopic signals? How can we control the directionality of energy carrier flow?

*Speaker

Thermal metrology for phase-change non-volatile memories

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The thermal characteristics of the phase change materials as well as the nearby dielectric materials affect the phase change memory's performance. In this study, we report on the thermal conductivity of the dielectric SiN and the nitrogen doped GeSbTe using 3ω method and show that the value is consistent with earlier measurements using Raman thermometry.

Keywords: Phase change materials, Thermal Conductivity, Thermal Boundary Resistance, 3ω method, Raman thermometry

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Nanothermometry-Guided In Situ Decoding of Perovskite Solar Cell Degradation under Optical Stress

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The thermal behavior of functional materials is closely linked to their stability and performance, particularly in optoelectronic devices such as perovskite solar cells (PSCs). In these devices, temperature variations at critical interfaces are both influenced by operational and environmental conditions and can, in turn, affect material properties, charge transport, and long-term stability. While PSCs have demonstrated remarkable power conversion efficiencies,(1) their long-term stability remains a major challenge, (2–6) with degradation mechanisms strongly influenced by local environmental conditions, including heat accumulation at buried interfaces. Understanding and monitoring these localized thermal dynamics in situ is therefore essential for unraveling degradation pathways and improving PSC stability. In this work, we introduce a new in situ methodology that harnesses the nano-thermometric properties of embedded upconversion nanoparticles (UCNPs) placed at the buried perovskite/hole transport layer (HTL) interface. This approach allows, for the first time, real-time tracking of local interfacial temperature evolution during light-induced accelerated degradation, while simultaneously monitoring the device's optical and photovoltaic performance. Applied to PSCs with different perovskite compositions, this technique reveals non-trivial thermal signatures and distinct degradation regimes correlated with structural and optical changes observed via ex situ characterizations. The results uncover a dynamic interplay between heat accumulation, phase transformation, and material decomposition, offering insights into the spatiotemporal evolution of PSC degradation.

Keywords: Nanothermometry, Perovskite solar cells, In situ degradation, Buried interface, Thermal evolution

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Systèmes de conversion

Influence of the solid initial surface charge on liquid-solid contact electrification

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Contact electrification and electrostatic induction are the core mechanisms behind Solid-liquid (SL) triboelectric nanogenerators (TENGs), which have gained tremendous attention for powering micro-scale devices in recent years. However, fundamental understandings of charge transfer within SL-TENGs remain relatively poor, limiting their optimized materials selection and device design. To move SL-TENGs beyond scientific curiosities, it is crucial to understand the electrification phenomenon. We used water droplets and polytetrafluoroethylene (PTFE) as a model system to examine how the film initial charge conditions influence the contact electrification of PTFE films and SL-TENG output voltage. Experimental characterizations and modeling revealed that the initial charge state of PTFE films greatly affects SL-TENG output voltage. Water, and other organic liquids, could not only lead to the appearance of negative charges on PTFE (aligning with the standard liquid-solid electrification model), but also neutralize them. This study demonstrates the importance of initial charge conditions in the contact electrification phenomenon.

Keywords: Triboelectricity, Liquid, solid contact electrification, Triboelectric nanogenerator, Initial conditions

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MEMS Design for Electrostatic Near-Limits Kinetic Energy Harvesting Under Simple Algorithm and Low Control Voltage

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This paper proposes simple control algorithm adapted for new MEMS electrostatic energy harvester designed for implementing the so-called Near-Limits technique using low control voltage.

Keywords: MEMS, kinetic energy harvesting, electrostatic, Near Limits.

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Eco-compatible cluster-polyoxometalate tandems for the production of hydrogen: from molecular assemblies to the device

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Green hydrogen, as an energy vector, holds the promise of a clean, cheap and sustainable energy. Using the most eco-friendly materials possible is a target to reach for the development of green photo-induced hydrogen catalytic systems for hydrogen evolution reactions (HER). However, to date, the most efficient photocatalysts reported in the literature contain noble metal like ruthenium or iridium as sensitizers. Beyond to be built from scarce metals, these systems suffer of a lack of stability that originates for instance of the photo-bleaching of organics components. In this context, we are currently investigating greener photoelectrocatalytic systems free of noble-metal or toxic elements for solar hydrogen production. These new photoelectrocatalysts associate a metal atom cluster (CLUS) and a polyoxometalate (POM) to form push-pull tandems, named CLUSPOMs.
In the CLUSPOM tandems, the cluster building blocks (M6Li8La6)2- (M=W, Mo; L=Ligands) acts as a robust photosensitizer. These are electron-rich molecular entities exhibiting very interesting optical properties(1),(2) and the ability to transfer electrons to other species(3) in the excited state, making them suitable for photocatalytic applications.

Polyoxometalates (POMs) are water-soluble metal-oxide discrete polyanions (e.g.(P2W18O62)6- and (PW12O40)3-), displaying the ability to exchange reversibly several electrons, making them highly relevant for catalytic processes involving multi-electrons transfers. Sulfur-functionalized POMs (i.e. (AsW15O53Mo3S4(H2O)3)7- and ((PW11O39)Mo3S4(H2O)3OH)8-), namely polyoxothiometalates, are proven to be among the most efficient POM-based HER photoelectrocalaysts reported so far in the literature(4),(5).

The association of clusters and POMs offers the prospect of the development of new high-

*Speaker

performance photoelectrocatalytic systems for hydrogen production. In this talk, we will present the first steps of the design and the characterization of photoelectrodes based on the association of clusters and polyoxometalates.

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(3) Anam F., Smortsova, Y., Falaise, C., et al. *Chem. Commun.*, 2023, **59**, 10988-10991 **DOI: 10.1039/D3CC03334A**

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Transport

Phonon lifetime in doped crystals

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Since the seminal work of Klemens, Talwar and Tamura in the early eighties, the increase of computing power and development of ab-initio methods have allowed the simulation of phonon interaction with scattering centers (substitutions, vacancies, stacking defects, es. works by Stewart and Mingo) with great accuracy. However, little improvement has been made to the theory beyond the initial real-space supercell formulation, which is based on a single-defect perturbation, which can be non-convergent in perturbation theory.
We have developed a new reciprocal space formulation, which models the scattering center as a phonon-phonon interaction potential V(q,q') that can be Fourier interpolated to any q and q'. In this framework, the defect concentration is introduced in a natural way, and the Tamura model appears as the natural limit V=0. The lifetime contribution can be combined with intrinsic anharmonicity for thermal transport, while the calculation of the full phonon self-energy allow the simulation of the full vibrational spectra.

The formulation can further be extended to lattice defects that do not conserve the number of atoms: defects and inclusions. We will present the theory development and application to some simple cases and materials

Keywords: phonon, simulation, doping, transport, anhamronicity

*Speaker

Machine Learning Guided Discovery of Extreme Thermal Conductivity in Si/Ge Superlattices

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Abstract- We present a combined computational and machine learning (ML) framework to study thermal conductance (G) and, as a result, lattice thermal conductivity () in Si/Ge superlattices. Using a combination of first principles and non-equilibrium Green's function (NEGF) simulations as training data, we construct and train neural networks for rapid prediction. Our results reveal that interface engineering can yield both ultra-low (phonon localization) and unexpectedly high (enhanced coherent transport in select random configurations). Our findings highlight design routes to achieve both ultra-low , relevant for nanocoolers, and ultra-high , desirable for heat dissipation in electronic devices.

I. INTRODUCTION

The rapid growth of artificial intelligence and data-intensive workloads has dramatically increased the energy demand and, consequently, the power density of modern processors. This surge results in significant heat generation and the formation of localized hotspots, which degrade device performance, reduce energy efficiency, and compromise reliability. While conventional cooling methods, such as fans, heat sinks, and liquid cooling, effectively remove heat at the system level, they remain inadequate for managing heat flow at the nanoscale, where phonons are the primary heat carriers in semiconductors and dielectrics. Within this context, two complementary strategies are essential: (i) employing materials with high for passive spreading and dissipation of heat away from hotspots; and (ii) utilizing thermoelectric nanocoolers that actively pump heat away and require low to suppress parasitic heat leakage. Engineering nanostructures that span and control these extremes of is therefore central to the advancement of next-generation electronics and energy devices.

Si/Ge superlattices represent a versatile platform to address this dual challenge. With their CMOS compatibility, industrial relevance, and tunable phonon transport properties, they provide a unique opportunity to design structures spanning from incoherent (strongly scattered)

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to coherent (wave-like) phonon transport regimes. Through periodic, graded, and random layer configurations (Fig. 1), it is possible to engineer interface density and disorder, thereby enabling control over lattice thermal conductivity across wide extremes (1). However, systematically exploring this design space with accurate first principles simulations is computationally expensive. To overcome this, we combine atomistic phonon transport simulations with neural network models, enabling efficient discovery of Si/Ge superlattices tailored for application-specific, extreme thermal transport properties (2).

II. Model and discussions

We construct datasets of thermal conductance, G, and thus, the lattice thermal conductivity, using atomistic NEGF-based phonon transport simulations of Si/Ge superlattices with varying interface numbers and thickness distributions (periodic, graded, random) (Fig. 2). The harmonic force constants for Si are obtained from first-principles calculations performed using Quantum ESPRESSO, serving as input for our in-house NEGF phonon transport tool. For simplicity, we assume Ge shares the same lattice and force constants as Si, differing only in atomic mass (1). The resulting material arrays are used as input features for our machine learning model. Before entering the neural network, principal component analysis (PCA) is used to reduce model complexity and avoid training with non-relevant features. A neural network is then trained to predict G/ (Fig. 3). The trained model efficiently identifies superlattices with extreme values, which we validate through direct transport simulations. Results reveal a competition between coherent and localized phonon modes depending on the interface arrangement.

III. Conclusion

Our ML-guided study (Fig. 4) reveals design principles for achieving both minimum and maximum in Si/Ge superlattices, with direct relevance to thermoelectric cooling and nanoscale heat dissipation.

Acknowledgment

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(2) Y. Luo, M. Li, H. Yuan, H. Liu, and Y. Fang, "Predicting lattice thermal conductivity via machine learning: A mini review," *npj Comput. Mater.* vol. 9, p. 4, 2023.

FIGURE 1: Schematic representation of the considered Si/Ge superlattices for simulations using a combination of first principles and NEGF.

FIGURE 2: Schematic representation of heat flow across the device (random) consisting of Si/Ge. Blue and red correspond to Si and Ge atoms, respectively.

FIGURE 3: Schematic representation of ML workflow.

FIGURE 4: Performance of machine learned model for thermal conductance (G). The corresponding lattice thermal conductivity () can be calculated by taking the product of G and the length of the superlattice.

Keywords: Thermal conductivity, Machine learning

First principles calculations of thermal transport at metal/silicon interfaces: Evidence of interfacial electron-phonon coupling

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With the increasing miniaturization of electronic components and the need to optimize thermal
management, it has become essential to understand heat transport at metal-semiconductor interfaces. While it has been recognized decades ago that an electron-phonon channel may exist at metal-semiconductor interfaces, its existence is still controversial. Here, we investigate thermal
transport at metal-silicon interfaces using the combination of first principles calculations and nonequilibrium
Green's function (NEGF). We explain how to correct NEGF formalism to account for the out-of-equilibrium nature of the energy carriers in the vicinity of the interface. The relative corrections to the equilibrium distribution are shown to arise from the spectral mean free paths of silicon and may reach 15%. Applying these corrections, we compare the predictions of NEGF to available experimental data for Au-Si, Pt-Si and Al-Si interfaces. Based on this comparison, we infer the value of the electron-phonon interfacial thermal conductance by employing the twotemperature
model. We find that interfacial thermal transport at Au-Si interfaces is mainly driven by phonon-phonon processes, and that electron-phonon processes play a negligible role at this interface.
By contrast, for Al-Si interfaces, we show that phonon-phonon scattering alone can not explain the experimental values reported so far, and we estimate that the electron-phonon interfacial
conductance accounts for one third of the total conductance. This work demonstrates the importance of the electron-phonon conductance at metal-silicon interfaces and calls for systematic
experimental investigation of thermal transport at these interfaces at low temperatures. It opens

*Speaker

also the door for the building of an accurate model to predict the conductance associated to the interfacial electron-phonon channel.

Keywords: transport de chaleur interfacial, couplage électron phonon, calculs premiers principes

Development of reference samples for calibrating resistance and current measurements in conductive probe atomic force microscopy

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As technological progress continue to push back the limits of device manufacturing to incredibly small scales, a commensurate development of measurement tools and methods is inevitable. Conductive probe atomic force microscopy (C-AFM) is a scanning probe microscopy technique widely used to measure currents and resistances at the nanoscale. Its popularity has recently increased due to the versatility of its applications in mainstream technologies such as memory, photovoltaics and semiconductors.
Despite the considerable contributions of C-AFM to understanding nanomaterials and nanodevices' properties, measurements have remained prone to numerous artifacts-inducing factors and restricted to qualitative comparisons. With the aim at making C-AFM measurements calibrated, reliable and comparable, we have recently developed the first standard reference sample for the calibration of the complete C-AFM measurement circuit over a resistance range of 9 decades, *i.e.* between 100 Ω and 100 GΩ. Measurement protocols using resistance mapping and current-versus-voltage (I-V) spectroscopic modes have also been drawn-up and the experimental, instrumental and environmental factors have been investigated to evaluate the complete C-AFM setup. We have shown that our developed multi-resistance wide-range standard sample allows a universal calibration of C-AFM measurements applicable to all available systems and enables the calibration of C-AFM with a combined relative uncertainty (given at one standard deviation) lower than 2.5% for resistances ranging from 10 kΩ to 100 GΩ (1).

In this work, we present the development of a second design of reference sample enabling easier access and improved accuracy to C-AFM measurements of resistance lower than 100 kW and a resistance range expanded to 1 TΩ. This new reference sample has also been designed to calibrate the complete C-AFM setup for current measurements over a range from 10 fA to 10 μA. We have investigated the influence of the AFM probes (materials, wear ...) on both resistance and current measurements and improved the calibration methods.

In addition to this hybrid calibration kit for C-AFM, we have manufactured and tested a third design of reference sample to calibrate C-AFM for very high resistance values, *i.e.* in the 100 TΩ range.

*Speaker

These recent developments pave the way for reliable quantitative measurements of resistances and currents at the nanoscale, which is expected to propel the understanding of the electrical properties of individual devices and components at the nanoscale.

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Simulation

Monte Carlo Modeling of Phonon Drag Effects on Thermoelectric Transport in Silicon Nanostructures

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A silicon-based nanofilm is examined using a self-consistent electron–phonon transport model. In this approach, an ensemble Monte Carlo solver for electrons is coupled with a phonon bath of non-uniform temperature, allowing us to incorporate the phonon drag effect. This simulation tool enables the study of thermoelectric properties in doped silicon nanostructures with varying sizes and interface types. In the present work, the total Seebeck coefficient of silicon nanofilms is analyzed under the influence of temperature, device length, and carrier concentration.

*Speaker

Gapless Dirac states in a strong spin-orbit coupling material

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The quest for high-performance thermoelectric materials is driving intense research on low-dimensional systems where electronic topology and strong spin–orbit coupling (SOC) can dramatically enhance transport properties. Two-dimensional (2D) Dirac states are particularly appealing because their linear dispersion favors high carrier mobility, yet they are generally fragile and tend to gap out under perturbations such as SOC. In graphene, for example, the SOC is weak, which allows the persistence of gapless Dirac states; otherwise, graphene would have been a quantum spin Hall insulator (1,2).
In this context, we investigate a 2D phase of bismuth, the α-phase, which hosts robust gapless Dirac cones despite its strong SOC. This metastable phase requires a supporting substrate; in our work, Au(111) is employed to stabilize it. The protection of the Dirac states arises from the nonsymmorphic symmetry of the lattice, offering a new route to realize symmetry-protected Dirac states in 2D systems.

Our results, developed within the framework of the ANR-NEXTOP (3) project on topological 2D materials for thermoelectric energy conversion, highlight how crystalline-symmetry protection can be exploited to engineer materials with both fundamental topological interest and promising thermoelectric performance.

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Realization of symmetry-enforced two-dimensional dirac fermions in nonsymmorphic alpha-bismuthene. ACS Nano, 14(2):1888–1894, 2020

(3) https://anr.fr/Projet-ANR-22-CE09-0035

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Keywords: Thermoelectric, 2D systems, topology, strong spin, orbit coupling, Dirac states.

Exact heat flux formula and its spectral decomposition in molecular dynamics for arbitrary many-body potentials

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In this work, we present an exact framework for calculating heat flux and its spectral decomposition in Molecular Dynamics (MD) for general many-body potentials. Our approach overcomes several shortcomings and limitations of previous methods, enabling accurate computational studies of thermal properties across a wide range of many-body systems within MD. We validated the framework through Green-Kubo (GK) and Non-Equilibrium MD (NEMD) simulations on various 2D and 3D materials, using the Tersoff and Stillinger–Weber (SW) potentials as test cases. Additionally, we computed the spectral decomposition of the heat current in monolayer graphene (1LG) and MoS for systems of varying lengths. The results demonstrate that our method consistently produces heat currents in agreement with the thermostat current in NEMD, whereas earlier implementations often yield poor estimates of thermal conductivity in both GK and NEMD simulations for both 2D and 3D systems. Furthermore, the decomposition of the heat current provides valuable insight into the contributions of different phonon modes to thermal conductivity and its length dependence. Our methodology has been implemented in the widely used LAMMPS package for the Tersoff and SW potentials, and can be readily extended to most other many-body MD potentials.

Keywords: Heat Flux, LAMMPS, Spectral Decomposition, Many body potentials, NEMD, Green Kubo, Molecular Dynamics

*Speaker

Rayonnement et transport thermique

Decoupling thermoelectric coefficients of multilayer graphene by nanomeshing

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Nanostructuring materials at small scales enables control over their physical properties, revealing behaviors not observed at larger dimensions (1). This strategy is particularly effective in two-dimensional (2D) materials, where surface effects dominate, and is particularly promising for energy conversion and thermal management (2).
In a recent work, we have uses multilayer graphene (4-6 nm thick) as a test platform to study the effect of nanomeshing on its thermoelectric coefficients (3). The nanomesh consists of a hexagonal array of holes, with a measured diameter and neck-width of $\sim$ 360 nm and $\sim$ 160 nm, respectively. The multilayer graphene is integrated into field-effect transistor-like devices supported by hexagonal boron nitride (hBN), allowing simultaneous electric and thermoelectric measurements, with nanomeshing applied to only part of the material. We use modulated thermoreflectance4 to investigate thermal transport in equivalent nanomeshed and pristine graphene flakes. We have revealed that the nanomesh geometry suppresses thermal transport without significantly impacting charge transport, highlighting the different scattering lengths of phonons and electrons while enhancing the thermopower response. We observe a twofold improvement in the device power factor, PF = S$\hat{}$2σ (with S the Seebeck coefficient and σ the electrical conductivity), at room temperature, along with a nearly threefold reduction in thermal conductivity k. These results show that nanomeshing can significantly decouple the thermoelectric coefficients of multilayer graphene, paving the way for novel engineering solutions to achieve similar control over a wider set of 2D materials.

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*Speaker

Keywords: thermoelectricity, graphene, nanostructuring

Interplay of Electron–Phonon and Impurity Scattering in the Thermal Transport of Heavily Doped Silicon

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A detailed understanding of the scattering mechanisms that limit heat transport in doped semiconductors is essential for effective thermal management in nanoelectronics and for the design of high-performance thermoelectric devices. While electron-phonon (el-ph) and electron-impurity interactions are well-studied in the context of charge transport in semiconductors (1,2), research on the impact of el-ph and phonon-impurity (ph-imp) interactions on phonon lifetimes and, consequently, on lattice thermal conductivity, remains rare. In this presentation, I will show our recent work, which explores the influence of el-ph and ph-imp scattering on the lattice thermal conductivity of heavily doped silicon (3), combining density functional theory-based first-principles simulations and 3-omega measurements. Our findings show that at moderate carrier concentrations (_˜10^{1} cm^3) and room temperature, phonon scattering by electrons is the main mechanism behind the reduction of thermal conductivity in doped silicon. However, at lower temperatures or higher doping levels (_˜10^{21} cm^3), both el-ph and ph-imp scattering significantly contribute to reducing the lifetimes of low-frequency phonons, which leads to further decreases in the thermal conductivity of doped silicon. Our results show good agreement with experimental thermal conductivity data for silicon across the full range of doping levels and temperatures.

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Keywords: Heat transport, Electron, Phonon and impurity, phonon scatterings, Doped Silicon,

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Density Functional Theory, 3omega measurements

Anomalous Temperature-Dependent Thermal Transport in Crystalline Polyethylene Driven by Strong Anharmonicity

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Thermal conductivity typically decreases with increasing temperature along the three principal crystalline directions, primarily due to enhanced phonon anharmonicity. In this work, we conducted a comprehensive first-principles investigation of thermal transport in crystalline polyethylene by solving the Wigner transport equation. It is found that the thermal conductivity of crystalline polyethylene decreases along the chain direction, but increases nearly linearly in the out-of-chain directions. This anomalous contrasting behavior stems from the dominance of particle-like transport along the chain and wave-like transport in the out-of-chain directions. The strong anharmonicity facilitates phonon tunneling between high- and low-frequency modes in the out-of-plane directions.

Keywords: Thermal conductivity, Crystalline polyethylene, Particle, like thermal transport, Wave, like thermal transport, First, principles calculations

*Speaker

STUDY OF SELF-HEATED RESISTIVE PROBE WEAR IN SCANNING THERMAL MICROSCOPY (SThM)

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Development of miniaturised electronic devices is partly based on the use of nanomaterials (nanowires, 1D and 2D materials) which can have high aspect ratio. In such devices, thermal management issues become prominent (overheating, local hot spots). In order to improve the thermal management of electronic components, manufacturers require reliable thermal properties measurements at nanoscale.
One of the suitable techniques to perform measurements of thermal properties at nanoscale is the Scanning Thermal Microscopy (SThM) technique (1), (2). The sensor is a resistive probe. In active mode (self-heating of the probe by Joule effect), the probe acts both as a heating source and as a temperature sensor. When the "hot" probe is in contact with the surface of a "cold" sample, heat transfer occurs between the probe and the sample. This heat transfer depends, among other parameters, on the thermal conductivity of the material and induce a variation of the probe temperature and, as a result, a variation of its electrical resistance . The determination of the studied material from the measured is possible through a calibration process of the dedicated probe and by following the measurements protocols defined in ref (3). Unfortunately, these probes are subject to wear that can significantly decrease the reproducibility of measurement and it is necessary to repeat the calibration process to keep the trueness of measurements.

In this contribution, the drift of the electrical resistance value of a resistive Pd type SThM probe has been studied, for several months. The probe was used in active mode and various types of tests and measurement campaigns were conducted (changes in electric current level, mapping of surfaces with high topography, numerous landings of the probe on the surface of various samples). Depending on the measurement conditions, the probe was subjected to different sources of wear (electrical shocks or variations, mechanical bending or torsion, erosion or flattening of tip apex). In addition, studies of the electrical response of Pd probes placed in thermal enclosures have been performed in order to check the influence of the operating temperature and the level of current on the wear of the probe. Analysis of the results enabled us to identify the main factors involved in probe wear (level of current and operating temperature). Finally, we propose recommendations to mitigate the impacts of the identified factors involved in probe wear and to improve the reliability and reproducibility of the measurements made with

*Speaker

Pd-type resistive probe in active mode.

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Elaboration

Liquid-Processed Metal Oxide and Chalcogenide Thin Films for High-Performance 3D Micro-Supercapacitors

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The rapid evolution of miniaturized electronic systems-including autonomous sensors, biomedical implants, and IoT devices-has created an urgent demand for integrable microscale energy storage solutions that combine high energy and power densities with long-term reliability (1). In this context, this study presents a scalable, low-temperature, solution-based strategy for the integration of nanostructured active materials-namely the metal oxides TiO2 and MoO3, and the chalcogenide MoS2-on both two-dimensional (2D) and complex three-dimensional (3D) silicon substrates, with and without vertical graphene (VG) interlayers. The VG architecture, fabricated by plasma-enhanced chemical vapor deposition, serves as a highly conductive and accessible backbone, promoting efficient charge transport across the electrode–electrolyte interface. All active materials were synthesized through soft-chemistry approaches, including sol-gel and colloidal routes, and deposited by spin-coating. This method enables homogeneous, crack-free, and conformal thin films on non-planar geometries without relying on vacuum processing or high-temperature sintering (1-3). Particular emphasis was placed on the fabrication of anatase-phase TiO via controlled hydrolysis of titanium alkoxides in alcoholic media. The process offers fine control over film thickness (20–300nm), porosity, and surface uniformity (1). Cross-sectional SEM imaging (Fig.1) reveals the conformal envelopment of VG flakes by the TiO2 layer throughout the 3D silicon scaffold, while in situ EDX mapping confirms the chemical homogeneity and absence of exposed regions.

MoO3 thin films were synthesized via a liquid-phase route involving peroxide-mediated dissolution and complexation in 2-methoxyethanol, yielding α-MoO nanocrystals with lamellar morphology and thicknesses of approximately 60nm for four spin-coated layers. XRD analyses confirm the formation of the orthorhombic α-phase, while SEM reveals crystallites ranging

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from 100 to 490nm in lateral size. The combination of TiO2 and MoO3 in a layer-by-layer (LBL) configuration was investigated to synergize the high structural stability of TiO with the high pseudocapacitive contribution of MoO3, leading to enhanced charge storage performance through interfacial coupling (4).
MoS2 was prepared by various soft-chemistry approaches-including liquid-phase exfoliation, hydrothermal growth, and spin-coating from thiomolybdate precursors-allowing fine control over the morphology, sheet thickness, and chemical composition. The integration of MoS into the electrode stack broadened the operating potential window and introduced additional pseudocapacitive behavior due to reversible ion intercalation and surface-based charge storage processes (5).
Electrochemical characterization performed by cyclic voltammetry and galvanostatic charge-discharge highlights the synergistic effects of vertical graphene and nanostructured oxides, with a marked enhancement in areal capacitance for TiO2@VG and LBL TiO2/MoO3 architectures compared to planar or single-material electrodes. These results validate the effectiveness of this solution-processed, multilayer integration approach for the development of robust, energy-dense micro-supercapacitor platforms (6).
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Keywords: Metal oxide, Chalcogenide, Thin films, Micro, supercapacitors, Liquid, processed, 3D electrodes, TiO2, MoO3, MoS2

Van der Waals Epitaxy of 2D material-based heterostructures on various crystalline substrates

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The crystal structure of a solid largely dictates its electronic, optical and mechanical properties. Engineering crystalline symmetry is not straightforward due to the strong covalent/ionic bonds in bulk crystals, however the discovery of new phases and phenomena (polytype, hybridization, superconductivity, ferroelectricity, moiré, etc...) in two-dimensional materials-has been based on the ability to rationally control crystal structures through materials synthesis, strain engineering or heterostructuring of van der Waals bonded materials. It is due to the ease of interlayer symmetry operations, of layer distance control and of layers slippage. This 2D anisotropy is particularly important in the emerging fields of 2D thermal phonons (1,2). 2D materials have a record thermal anisotropy (ratio between in plane and out of plane of 900), with room for improvement. (3) In-plane thermal conductivity in 2D goes from 5000 W.m-1.K-1 in graphene or thin graphite (4) to very low values, _˜ 0.1 Wm-1.K-1. (5) The vertical conductivity in a heterostructure can be reduced to 0.009 Wm-1.K-1. (6) behaving like a perfect insulator. Thus, 2D heterostructures can be used as a near ideal heat spreaders in integrated circuits, that can eliminate hot spots along the direction of the fast axis and provide thermal insulation along the slow axis. Within these perspectives, the epitaxial engineering of 2D heterostructures is an evidence.

As an example, we demonstrate the quasi-van der Waals epitaxy of a WSe2/PtSe2 heterostructure on Se-terminated W(110) substrate, as evidenced by the alignment of the () hexagonal LEED pattern of both WSe2 and PtSe2 without any moiré effect, while Raman spectroscopy showcases both materials vibration modes. Besides, the combination of Raman spectroscopy and ARPES measurements on WSe2 bilayer strongly evidence the dominant formation of the 3R polytype. We further demonstrate the epitaxial growth of a WSe2/HfSe2 heterostructure on Se-terminated GaP(111) substrate with clear p-n junction type II band alignment and strong evidence of van der Waals interfaces between the three materials (7).

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Hommage à Natalio Mingo

Thermal transport simulation at sub-Kelvin by Finite Element Non-Equilibrium Green's Function

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Simulating heat transport in the sub-Kelvin regime is essential for thermal management in emerging technologies such as quantum computing. At these cryogenic temperatures, phonon transport becomes ballistic and phase-coherent, rendering classical approaches like Fourier's law invalid. The Non-Equilibrium Green's Function (NEGF) formalism for phonon transport, pioneered by Mingo and Yang in 2003 (1), provides an accurate quantum mechanical framework to capture these effects. When integrated with the finite element (FE) method, NEGF enables device-scale simulations of thermal transport that can be directly compared with experimental results for quantum thermal conductance (2,3). This combined approach-referred to as FENEGF-is now being actively applied to address the pressing thermal challenges in quantum computing systems.

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*Speaker

Thermal transport in semiconductors: from coherent to strongly anharmonic regime

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In this talk, I will reflect on my collaborative work with Natalio Mingo on lattice thermal transport in disordered systems (1,2,3). This collaboration sparked many research questions that I have continued to pursue to this day, including studies of lattice thermal transport in strongly anharmonic systems, which I will also discuss (4,5).

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*Speaker

Mingo's atomistic Green's function approach to nanoscale thermal transport and its comparison with experiments

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Natalio Mingo has dedicated his scientific career to the study of thermal transport for over 20 years. He pioneered the use of an atomistic Green's function approach to calculate phonon transport properties in dielectric nanostructures, beginning with his seminal 2003 paper co-authored with L. Yang.

*Speaker

Invite : T. Sohier

Ab-initio modeling of electron-phonon scattering in 2D heterostructures

Thibault Sohier * [1], Francesco Macheda

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2D materials have shown fascinating fundamental physics as well as exciting technological prospects, from transistors to integrated optoelectronics. Many applications rely on the ability of the 2D material to conduct electrons efficiently. At room temperature, this is mostly limited by the scattering of electrons by phonons. A clear understanding of electron-phonon scattering, along with predictive ab initio simulations, are then key to design performant and energy-efficient devices. Most device designs with 2D materials involve encapsulation, whereby an operative 2D material is sandwiched in between several layers of a protective material.
Such stacking of 2D materials into van der Waals heterostructures implies the emergence of interlayer interactions, modifying electronic scattering in a given layer. We develop an efficient ab initio approach to compute the electrodynamic response of 2D heterostructures, including long range Coulomb interactions between electrons, polar phonons, and plasmons. We extract electron scattering from this model and solve a system of coupled Boltzmann transport equations for electrons and electrodynamic modes. This accounts for non-trivial momentum exchanges such as the so-called phonon drag. We study the effects of remote electron-plasmon-phonon couplings on the electronic transport properties of 2D materials. We also show that a dynamical treatment of electronic screening has a significant impact on the mobility of doped semiconductors with a Fermi level around the band edge. Indeed, polar phonons dynamically coupled with electron-hole excitations scatter momentum differently than the standard polar phonons, whether bare or statically screened.

*Speaker

Invite : E. Baudin

Electroluminescence and Energy Transfer in hBN-encapsulated Graphene Transistors

Emmanuel Baudin * [1]

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In this talk, I will present our recent discovery of graphene's electroluminescence in the middle infrared. Electroluminescence is the phenomenon by which a material emits light in response to the passage of an electrical current. In solids, it is the prerogative of semiconductors and related organic materials, and it results from the radiative recombination of electrons and holes. We investigate high-mobility graphene field-effect transistors encapsulated in hexagonal boron nitride (hBN) at ambient conditions. Despite the semimetallic nature of graphene, which theoretically precludes electroluminescence, we observe this phenomenon due to (i) inefficient non-radiative carrier relaxation and (ii) a unique carrier injection mechanism specific to 2D semimetals: Zener-Klein tunneling.

Our results reveal two important consequences of graphene electroluminescence. First, it leads to mid-IR emission in the far field. Second, it significantly affects the energy transfer within the hBN-encapsulated heterostructure. Using far-field mid-IR spectroscopy, we demonstrate the far-field electroluminescence of graphene at 6.5 μm, made possible by the elastic scattering of hyperbolic phonon polaritons (HPhPs) of hBN at heterostructure discontinuities. We quantify the associated radiative energy transfer using mid-IR pyrometry of the substrate receiving the thermal energy.

Surprisingly, we find that radiative energy transfer is reduced in hBN with nanoscale inhomogeneities, revealing the crucial role of the electromagnetic environment and opening interesting technological possibilities.

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*Speaker

Invite : G. Despesse

Les matériaux piézoélectriques au service de l'électronique de puissance

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Ce papier propose une introduction à la conversion de puissance utilisant des résonateurs piézoélectriques comme moyen de stockage temporaire au lieu des inductances. Il s'agit d'une voie prometteuse du fait de la densité élevée d'énergie stockable par unité de volume de certains matériaux. Une densité de puissance de conversion de 5.7 kW/cm3 a été atteinte dans l'état de l'art avec du Niobate de Lithium avec un rendement $> 97\%$.

*Speaker

Invite : S. Matzen

Strain and light in micro-cantilevers based on ferroelectric thin films

Sylvia Matzen * [1], Stéphane Gable [1], Alexandre Zing [1], Thomas Maroutian [1], Guillaume Agnus [1], Philippe Lecoeur [1], Yousfi Said [2], Houssny Bouyanfif [2]

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Ferroelectrics (FE) are multifunctional materials, with coupled degrees of freedom, enabling to develop various innovative electronic devices with enhanced performance. The coupling between electric polarization and mechanical deformation leads to remarkable piezoelectric response with numerous applications in microelectromechanical systems (MEMS), such as actuators and sensors, whose archetypical geometry is the micro-cantilever structure. While the processing of thin films on silicon is critical for integration purposes, epitaxial ferroelectric thin films attract considerable attention because of their often superior properties over polycrystalline thin films. However, nowadays, most of the devices integrate FE with toxic lead (such as the well-known Pb(Zr,Ti)O3 or PZT). In addition, they usually operate with electrical bias which requires a complex circuitry with electrical contacts into more and more miniaturized scale, with an energy consumption intrinsically related to Joule heating. The future development of high performance MEMS based on FE thin films requires thus to address two main challenges: (i) finding alternative environmental friendly materials and (ii) explore new approaches to control strain in FE with better energy efficiency.
In this talk, recent research results will be presented trying to address these two aspects.

The first part will be focused on lead-free BiFeO3 thin films epitaxially grown on a SrRuO3/SrTiO3-buffered Si substrate and patterned into micro-cantilevers. The devices demonstrate excellent ferroelectric response and larger electromechanical performance than that of state-of-art piezoelectric cantilevers (including PZT), which can be further enhanced by the flexoelectric effect. These results show that BiFeO3can be a promising alternative for the development of piezoelectric MEMS that currently incorporate conventional piezoelectric materials from the lead-based perovskite family.
The second part will show the capability to control optically the strain in MEMS by using the photostriction mechanism (the non-thermal generation of strain). Photo-induced actuation of micro-cantilevers based on PZT ferroelectric thin films epitaxially grown on a (La,Sr)MnO3/SrTiO3-buffered Si substrate will be reported. This optical control of the strain in ferroelectrics could bring many advantages in comparison with traditional electrical control, by providing a wireless remote control, at lower energy consumption and faster time scale. More generally, this approach could have important implications for the light-mediated engineering of materials and devices functionalities.

*Speaker

Invite : R. Messina

Focusing of near-field heat flux radiated between a tip and a substrate for heat-assisted magnetic recording applications

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The development of fluctuational electrodynamics and the discovery that radiative heat flux can be strongly amplified in the near field have paved the way to several applications including heat-assisted magnetic recording (HAMR). In HAMR, a small surface area of a magnetic material is heated to raise its temperature close to the Curie temperature, where its magnetic coercivity is weak. Then by applying a magnetic field a new magnetic state can be recorded inside the material. Achieving high information densities requires the confinement of heat to nanoscale regions, ideally approaching the superparamagnetic limit of tens of nanometers.
In this work we address the spatially resolved near-field radiative heat transfer between a nanoparticle (simulating a tip) and a substrate in the fluctuational-electrodynamics framework within the dipolar approximation and explore two strategies both to enhance heat transfer and to spatially focus it.

In the first part, we consider the radiative heat transfer between a magneto-optical particle (whose optical properties can be manipulated by applying a magnetic field) and a substrate. We study the maximum of the Poynting vector below the nanoemitter and its Full Width Half Maximum (FWHM) as a function of the applied magnetic field for different radii of the nanoparticle. The results highlight a non-monotonic behavior, according to which the maximum Poynting vector (FWHM) first increases (decreases) as a function of the applied field, then decreases (increases), by reaching values even below (above) the reference one for vanishing field. This highlights the existence of an optimal scenario for which not only is the local heat flux quantitatively increased, but it is also more focused on the surface of the substrate. These results are interpreted by an analysis of the flux spectral properties and frequencies of resonant surface modes in the nanoparticle-substrate system.
In the second part, we consider the configuration of a tip made of a polar material and address the role played by a thin film of polar material placed on the underlying substrate. We show that this can also lead to a substantial enhancement and spatial focusing of the radiative heat flux. The influence of the probe–substrate separation, film thickness and substrate permittivity is analyzed, revealing that the effect originates from near-field interactions governed by the interplay between film-induced modifications of electromagnetic mode dispersion and the distance-dependent coupling strength. Our results highlight a viable route toward the active control of local radiative heat transfer at the nanoscale.

*Speaker

Invite : J. Sjakste

Coupled dynamics of hot carriers and phonons: describing time-resolved spectroscopy and transient transport with real-time propagation of carrier distributions.

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In recent years, computational approaches which couple density functional theory (DFT) - based description of the electron-phonon and phonon-phonon scattering rates with the Boltzmann transport equations (BTEs) have been shown to obtain the electron and thermal transport characteristics of many 3D and 2D semiconductors in excellent agreement with experimental measurements (1,2). Moreover, progress in time-dependent computational approaches, as well as progress in time-resolved spectroscopy experiments allows unprecedented insight into coupled dynamics of hot carriers and phonons (3).
After discussing relaxation regimes of photoexcited carriers in semiconducting materials (3), I will present our recent work on coupling of *ab initio* description of carrier-phonon scattering with stochastic Monte Carlo method for BTEs (4). Our approach allows to describe both transient transport characteristics and photoexcited carrier relaxation, in agreement with time-resolved ARPES. Finally, I will present our recent collaborative work on coupled hole and phonon dynamics in photoexcited germanium, which was studied by time-resolved Raman spectroscopy as well as by DFT calculations coupled with time-dependent two-temperature model. We will show that our time-dependent model based on DFT data can describe the observed changes in temperature of Raman-active optical modes, which are due to energy transfer from photoexcited holes to phonons, in excellent agreement with experiment (5).

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(4) M. Ghanem et al, in preparation (2025)
(5) G. Raciti et al, arXiv:2508.10544, submitted (2025)

*Speaker

Invite : J. Maire

Photothermal heterodyne imaging for 3D thermal microscopy

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To understand heat transfers or resolve underlying geometrical features in complex system, obtaining three-dimensional temperature measurements is a powerful source of information. Here we present the photothermal heterodyne imaging techniques based on the temperature dependent variations on the optical index. We combine this technique with laminography, a generalized version of computed tomography, and demonstrate a reconstructed 3D temperature field induced by a laser in a glass wafer.

*Speaker

Invite : M. Almanza

Réfrigération et matériaux électrocaloriques

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Ce papier propose une introduction à la réfrigération à partir de matériaux électrocaloriques (EC). Il s'agit d'une voie prometteuse pour offrir des densités élevées de puissance froide, une bonne efficacité et qui soit adaptable à différentes échelles. La réfrigération électrocalorique permet de repenser les systèmes de réfrigération, mais elle se heurte aussi à plusieurs limitations. Nous proposons de discuter des récentes avancés et limitations en allant des matériaux aux systèmes.

*Speaker

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