Photon, Phonon, and Electron Transitions in Coupled Nanoscale Systems

745. WE-Heraeus-Seminar

19 - 23 September 2022

hybrid

at the Physikzentrum Bad Honnef, Germany

WILHELM UND ELSE HERAEUS-STIFTUNG

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 745. WE-Heraeus-Seminar:

The coupling between nanosized subsystems is of great importance from the viewpoint of basic research and, not less important, in developing conceptually new devices. Even in low energy devices which are usually operated close to thermal equilibrium a coupling between two subsystems is caused by small differences in temperature leading to relatively large temperature gradients due to the small dimensions. For local temperature management, it might be desirable to avoid these gradients for draining waste heat or on the contrary to have as large as possible gradients during cooling of a local detector. These gradients cause a heat flow mediated by electrons and phonons which can be strongly influenced by interfaces reducing the coupling of the subsystems. Beside the heat conduction heat transport between subsystems can be mediated by photons or coupling through forces like the Casimir force. In the last years, there is a growing community from different disciplines interested in the different aspects of the heat transport phenomena by the different heat carriers in nanosystems down to molecular and even atomic scale. This seminar aims to bring together well-established experts, young academics, and graduate students (physicists, engineers, and chemists) working on experiments and theory of the photonic, phononic, and electronic transport properties in nanoscale systems. The program of the seminar will be organized in a series of lectures given by internationally recognized scientists in theoretical or experimental research. These lectures will give a pedagogical introduction into specific topics of the field and an overview of present development, new insights and novel result in theory as well as techniques and methods of measurements.

Scientific Organizers:

Prof. Dr. Achim Kittel	Universität Oldenburg, Germany E-mail: kittel@uni-oldenburg.de
PD Dr. Svend-Age Biehs,	Universität Oldenburg, Germany E-mail: s.age.biehs@uni-oldenburg.de

Introduction

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Registration:

Elisabeth Nowotka (WE Heraeus Foundation)
at the Physikzentrum, reception office
Sunday (17:00 h – 21:00 h) and Monday morning

Program

Program

Sunday, 18 September 2022

17:00 – 20:00	Registration	
18:00	*BUFFET SUPPER and informal get-together*	

Monday, 19 September 2022

07:30	*BREAKFAST*	
08:30	Scientific organizers	**Welcome words**
08:40 – 09:40	Matthias Krüger	**Mesoscopic theory and phenomena of fluctuational electrodynamics**
09:40 – 10:40	Philippe Ben-Abdallah	**Near-field heat transfer in many-body systems: from theory to applications**
10:40 – 11:10	*COFFEE & TEA*	
11:10 – 11:30	Minggang Luo	**Convection-type heat transfer behavior in the asymmetric nanoparticle chains via thermal photons**
11:30 – 11:50	Refet Yalcin	**Dependent scattering in thick and concentrated colloidal suspensions**
11:50 – 12:50	**Poster flashs**	
12:50 – 13:00	**Conference Photo** (in the front of the lecture hall)	
13:00	*LUNCH*	

Program

Monday, 19 September 2022

14:30 – 15:30	Mauro Antezza	**Torque and energy transfer in periodic systems**
15:30 – 16:30	Yannick De Wilde	**Probing the infrared thermal radiation of plasmonic patch antennas and dielectric microspheres**
16:30 – 17:00	*COFFEE & TEA*	
17:00 – 18:00	Sheila Edalatpour	**Modeling radiative heat transfer at the micro/nanoscale using the thermal discrete dipole approximation**
18:30 – 19:30	*DINNER*	
19:30 – 21:00	**Poster session I**	

Program

Tuesday, 20 September 2022

07:30	*BREAKFAST*	
08:30 – 09:30	Zhenghua An	**Nanoscopic imaging of nonequilibrium electron transport by scanning near-field microwave and terahertz microscope**
09:30 – 10:30	Fabian Pauly	**Thermal conductance of single-atom and single-molecule junctions**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 12:00	Dvira Segal	**Theory of electronic noise and simulations of phonon transport in molecular-scale junctions**
12:00 – 12:20	Pascal Gehring	**Thermocurrent spectroscopy of Yu-Shiba-Rusinov states in single-molecule junctions**
12:20 – 12:40	Yury Kosevich	**tba**
13:00	*LUNCH*	

Program

Tuesday, 20 September 2022

14:30 – 15:30	Pierre Oliver Chapuis	**Near-field radiative heat transfer in thermophotovoltaics and thermophotonics**
15:30 – 16:30	Pramod Sangi Reddy	**Energy transfer and conversion in nanoscale gaps**
16:30 – 17:00	*COFFEE BREAK*	
17:00 – 17:20	Karthik Sasihithlu	**Extended Förster's theory to include dynamic effects in resonance energy transfer**
17.20 – 17.40	Roman Anufriev	**Phonon mean free path in Si and SiC nanostructures linked to their thermal conductivity**
17.40 – 18.00	Jean Spièce	**Thermal transport in twisted 2D materials**
18:30 – 19.30	*DINNER*	
19.30 – 21.00	**Poster session II**	

Program

Wednesday, 21 September 2022

07:30	*BREAKFAST*	
08:30 – 09:30	Vera Musilova	**Effect of superconducting transition on near field heat transfer**
09:30 – 10:30	Bong Jae Lee	**Near-field thermal radiation and photovoltaic energy conversion**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 12:00	Shanhui Fan	**Non-reciprocal thermal radiation and energy harvesting**
12:00 – 12:20	Ivan Latella	**Solid-state pyroelectric system for near-field energy conversion**
12.20 – 12.40	Omar Jesús Franca Santiago	**Quantum Friction near nonreciprocal media**
13:00	*LUNCH*	
14:30 – 18:00	**Excursion**	
18:30	*DINNER*	

Program

Thursday, 22 September 2022

07:30	*BREAKFAST*	
08:30 – 09:30	Alejandro W. Rodriguez	**Limits on light–matter coupling at the nanoscale**
09:30 – 10:30	Nicolas Agrait	**Measuring the thermal and electrical conductance of atomic contacts using a novel hotwire-thermocouple scanning probe microscope**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 12:00	Karl Joulain	**Thermal rectification in quantum systems**
12:00– 12:20	Riccardo Messina	**Coupling between conduction and near-field radiative heat transfer in tip-plane geometry**
12:20 – 12:40	Florian Herz	**Generalized coupled dipole method for thermal far-field radiation**
13:00	*LUNCH*	

Program

Thursday, 22 September 2022

14:30 – 15:30	Elke Scheer	**Nonmonotonous temperature dependence of the thermopower of gold atomic contacts**
15:30 – 16:30	Samy Merabia	**Phonon transport at interfaces: from Kapitza resistance to single molecule junctions**
16:30 – 17:00	*COFFEE BREAK*	
17:00 – 17:20	Ilari Maasilta	**Recent progress in the theory of acoustic phonon tunneling across a vacuum gap between piezoelectric crystals**
17:20 – 17:40	Mauricio Gómez Viloria	**Heat transfer modelling in the crossover regime between conduction and radiation**
17:40 – 18:00	Yangyu Guo	**Atomistic simulation of phonon tunneling across metallic vacuum nanogaps**
18:30	*HERAEUS DINNER* *(social event with cold & warm buffet with complimentary drinks)*	

Program

Friday, 23 September 2022

07:30	*BREAKFAST*	
08:30 – 09:30	Sebastian Volz	**Surface phonon-polaritons as efficient heat carriers**
09:30 – 10:30	Mika Prunnila	**Phonon engineering for photodetectors and solid-state refrigerators**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 12:00	Eli Zeldov	**SQUID-on-tip nanoscale thermal imaging: Glimpse into dissipation in quantum systems down to atomic scale**
12:00 – 12:20	Sergey Sobolev	**Electron-phonon coupling in metals under ultrashort laser irradiation: two-temperature model**
12:20– 12:40	Raul Esquivel-Sirvent	**Non-Fourier time-harmonic photothermal heating by nanoparticles**
12:40 – 12:50	Scientific organizers	**Closing words**
13:00	*LUNCH*	

End of the seminar and departure

NO DINNER for participants leaving on Saturday; however, a self-service breakfast will be provided on Saturday morning

Posters

Posters

Hdeel Alamin	**CuO/TiO_2 nanocomposite photoanode for dye sensitized solar cell**
Mohamed Amara	**Radiative cooling of solar cells: detailed optoelectro-thermal modeling and influence of surface structuring**
Farzam Bahmani	**Localized edge states in radiative heat transfer**
Matthias Blaschke	**Mechanisms to tailor the phononic thermal conductance of molecular junctions unveiled by a genetic algorithm**
Jon Canosa Diaz	**Crystalline silicon based suspeded thermometry platforms: study of quantum phononic effects**
Giulio de Vito	**Phonon hydrodynamic transport in 2D materials**
Zhuoran Geng	**Heat transfer across vacuum gap by piezoelectric acoustic phonon tunneling**
Marvin Glittenberg	**A new sensor concept for scanning thermal microscopy**
Mario Graml	**Nonthermal photoinduced phase transition**
Yubin Huang	**Mapping local thermoelectric properties of MXenes via scanning thermal microscopy**
Mohamed Ibrahim	**Toward understanding thermal and electric properties of single molecular junctions and self-assembled monolayers**
Haiyan Lyu	**Novel probe for heat transport measurements in atomic and single molecule junctions**
Sunil Kumar Mahato	**Thin film diamond nano-photonics and its quantum application**
Alonso Marquez Hernandez	**NFRHT enhancement via external magnetic fields**

Posters

León-Alexander Martin	**GW + NEGF method for transport through nanostructures**
Ameneh Mikaeeli	**Correlation between thermal, optical and electrical conductivities in azo-dyes functionalized polymers**
Somayyeh Nemati	**Coupling function versus phononic density of states**
Mathis Noell	**Extinction of covered ellipsoidal nanoparticles**
Quentin Pompidou	**Measurement of thermal boundary conductance (TBC) by means of modulated-photo thermal radiometry technic (M-PTR)**
Sophie Rodehutskors	**Sphere probes for scanning thermal microscopy**
Tanja Schoger	**Universal Casimir interaction and its relevance for colloidal and biophysical systems**
Raza Sheikh	**Characterization of nanomaterials by means of spatially and frequency resolved photothermal radiometry**
Rahul Swami	**Electro- & opto-thermal measurements of low dimensional materials**
Timm Swoboda	**Spatially resolved thermometry on metal oxide RRAM devices by means of Scanning thermal microscopy**

Abstracts of Talks

(in alphabetical order)

Measuring the thermal and electrical conductance of atomic contacts using a novel hotwire-thermocouple scanning probe microscope

Nicolás Agrait
Department of Condensed Matter Physics-IFIMAC, Iniversidad Autónoma de Madrid Instituto Madrileño de Estudios Avanzados IMDEA-Nanociencia,

We study the thermal conductance gold atomic contacts with sizes ranging from one atom to several hundreds using a novel hotwire-thermocouple sensor consisting of two 5 µm Wollaston wires of Pt and Pt/Rh, respectively. We show that using a multifrequency scheme to measure simultaneously the thermovoltage at the tip and the average resistance of the wire, it is possible to measure heat conductances with sensitivities better than 0.1 nW/K. We also demonstrate that this sensor can be precisely calibrated in situ using the Peltier effect, obviating a detailed modelization of the probe.

Nanoscopic imaging of nonequilibrium electron transport by scanning near-field microwave and terahertz microscope

Zhenghua An[1,2,*], Qianchun Weng[3], Xiaodong Zhou[1,2], Huanyi Xue[1], Changhao Meng[1], Weikang Lu[1], Pingping Chen[3], Wei Lu[3], Susumu Komiyama[4]

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Conducting electrons in nanodevices exhibit strenuous interaction with hosting materials and eventually cause rich dynamic behaviors. Here we utilize two scanning near-field microscopes, i.e., scanning microwave impedance microscope (s-MIM) and scanning noise microscope at terahertz (SNoiM) [1], to study the nonequilibrium electron transport in semiconductor nanodevices. With s-MIM, the negative conductivity and hence microwave gain can be directly imaged at the nanoconstricted channel, which originate from the inverted population of satellite energy valleys. While the effective temperatures of the nonequilibrium transporting electrons can be mapped via SNoiM, providing in-depth pictures on electron transport dynamics. It is found that the nanoscopic profiles of electron temperature can be distinctively different from the hosting lattice [3,4] and the hot-phonon bottleneck effect [3] plays a remarkable role in the energy relaxation dynamics in transporting hot electrons. Our work suggests that s-MIM and SNoiM provide powerful tools for disclosing the nanoscopic information of nonequilibrium transport and might be helpful for the thermal management consideration in future optimization of electronic device performance.

References

[1] Qianchun Weng, *et al*, Science 360(6390), pp. 775-778, (2018)
[2] Xiaodong Zhou, *et al*, to be published.
[3] Qianchun Weng, *et al*, Nature Communications, 12, 4752(2021)
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Torque and energy transfer in periodic systems

M. Antezza

University of Montpellier, Laboratoire Charles Coulomb, Montpellier, France

We will present recent results on the theoretical study of the Casimir torque and radiative heat transfer between periodic systems made by lamellar diffraction gratings [1] and 2S arrays of nanoparticles [2]. Concerning the Casimir torque, we predict the existence of an anomaly close to zero rotation angle leading to huge vacuum induced torque in finite size systems. Concerning the radiative heat transfer we will show the existence of a rich phase diagram reflecting the different many-body to single body crossovers in 2D nanoparticle ensembles.

References

[1] Mauro Antezza, H. B. Chan, Brahim Guizal, V.N. Marachevsky, Riccardo Messina, Mingkang Wang, Phys. Rev. Lett. **124**, 013903 (2020)

[2] Minggang Luo, Junming Zhao, Linhua Liu, and Mauro Antezza, Phys. Rev. B **102**, 024203 (2020)

Phonon mean free path in Si and SiC nanostructures linked to their thermal conductivity

R. Anufriev[1] , J. Ordonez-Miranda[1,2], Y. Wu[1],

S. Volz[1,2], and M. Nomura[1]

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[2] *LIMMS, CNRS-IIS UMI 2820, The University of Tokyo, Tokyo 153-8505, Japan*

Knowledge of the mean free path (MFP) of phonons in nanostructures is essential for thermal and electric engineering in modern microelectronics. However, while the MFP in bulk materials is well known, its values in nanostructures made of technologically important materials remain overlooked.

In this work, we experimentally study the phonon MFP in Si and SiC nanostructures at different temperatures. Our measurements coupled with an analytical model reveal the MFP spectra of Si [1] and SiC [2] nanomembranes in the 4 - 400 K temperature range. The phonon MFP spectra measured in nanomembranes are orders of magnitude shorter than the spectra known for their bulk counterparts. Consequently, the measured thermal conductivity is several times lower than that in bulk and appears to be proportional to the smallest dimension of the nanostructures. To confirm this hypothesis, we measured the thermal conductivity of various Si and SiC nanostructures, including nanomembranes [1,2], nanowires [2,3], and phononic crystals [2,4]. Our experiments show that the thermal conductivity of all nanostructures scales proportionally to their dimensions. Using the Callaway-Holland model, we correlated the observed reductions of the thermal conductivity and MFP with the surface phonon scattering, which inherently limits the thermal conductivity at the nanoscale. Furthermore, the origin of the obtained thermal conductivity values for various nanostructures are explained via a mean free path analysis. This work thus provides a framework for predicting the thermal properties of arbitrary nanostructures, facilitating the thermal engineering in microelectronics.

References

[1] R. Anufriev et al., Physical Review B **101**, 115301 (2020)
[2] R. Anufriev et al., NPG Asia Materials **14**, 35 (2022)
[3] R. Anufriev et al., ACS Nano **12**, 11928 (2018)
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Near-field heat transfer in many-body systems: from theory to applications

Philippe Ben-Abdallah[1*]

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In this lecture I will discuss how to handle the radiative heat exchanges in many-body systems consisting of thermal emitters interacting in the near-field regime. After introducing the theoretical framework to describe these exchanges I will discuss some peculiarities of these systems compared to two body-systems and I will show how these effects can be used to control heat exchanges at nanoscale and to harvest the near-field energy confined close to a hot solid.

In the first part I will introduce a Landauer-like formula to describe the radiative heat exchanges in the general situation of multiterminal systems using transmission coefficients describing all pairwise interaction in these systems. I will deduce from this formalism a general rule linking these coefficients and I will show the possible existence of supercurrents at equilibrium in non-reciprocal systems. In the second part I will introduce an effect analog to the Coulomb drag (which exists between two electric conductors at close separation distance) and I will show how this effect can be used to locally control the temperature gradient in many-body systems. Next I will show how the cooperative interactions between several thermal emitters at different temperature can be used to focus and amplify the heat flux in their surrounding at a scale which is much smaller than the diffraction limit. In the third part I will show how heat can be locally pumped in many-body systems by modulated some physical properties, generalizing so to many-body systems the concept of radiative shuttling. Next I will show that non-trivial topological behaviors can appear in non-reciprocal systems and they give rise to new effects (thermomagnetic effects, and geometric pumping) which can be used to control heat flux at nanoscale. Finally I will present a three-body energy converter of the near-field energy and I will show that that this technology could be an efficient alternative to the near-field thermophotovoltaic converters at low temperature (T < 500K) and small temperature differences (ΔT~100K).

References

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9. I. Latella, S.-A. Biehs and P. Ben-Abdallah, Opt. Express, 29 (16) , 24816 (2021)
10. I. Latella and P. Ben-Abdallah, Sci. Rep., 11:19489 (2021)

Near-field radiative heat transfer in thermophotovoltaics and thermophotonics

C. Lucchesi[1], J. Legendre[1], M. Thomas[1], M. Piqueras[1], D. Cakiroglu[2], J.P. Perez[2], T. Taliercio[2], E. Tournié[2], R. Vaillon[2], **P.-O. Chapuis**[1]

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We first report on advances in thermophotovoltaics (TPV), which is close to photovoltaics (PV) – the cold side is a pn or pin junction acting as a PV cell - but where the emitter is a hot source instead of the sun. The efficiency is typically much higher than that of thermoelectrics and can reach 40% [1], but the output power density is usually lower due to the Planck/Bose-Einstein bound of thermal radiation. As a result, TPV has been mostly considered at high temperature. Recent progresses toward near-field operation, where the hot emitter is brought very close to the photovoltaic cell in order to stimulate photon tunneling, allow transferring much more heat than this bound and indicate that the W/cm^2 power density can be obtained for hot temperatures lower than 1000 K. We detail the recent experimental measurements [2,3] and analyze some pros and cons of near-field thermal radiation-based TPV devices [4].
A derived technology termed thermophotonics (TPX) [5], where the emitter is another pn or pin junction controlled electrically therefore acting as a light-emitting diode (LED), is also making progresses. The principle is to force the hot source to emit above the PV-cell bandgap, in order to convert efficiently, by means of electroluminescence. Theoretical reports of the imbalance between the LED consumption and the PV output power indicate that such technology is interesting for heat sources in the range 200-300°C, especially when hot and cold sides are brought in the near-field distance range [6].

References

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Probing the infrared thermal radiation of plasmonic patch antennas and dielectric microspheres

L. Abou-Hamdan[1,2], V. Krachmalnicoff[1], C. Li[1,2], J. Jaeck[2], N. Bardou[3], R. Haïdar[2], P. Bouchon[2], and Y. De Wilde[1]

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To probe the intrinsic electromagnetic response of single patch antennas, we have developed an infrared spatial modulation spectroscopy (IR-SMS) technique which allows to detect extremely small thermal radiation signals from sub-wavelength sized objects without background [1, 2]. We have applied it in combination with thermal radiation scanning tunnelling microscopy (TRSTM) [3] to measure both near-field images of the thermally excited electromagnetic modes on a patch antenna and the corresponding far-field thermal radiation spectra. When the dielectric spacer material of the patch is silica, different spectral resonances are associated with the same distribution of the electromagnetic field. This unexpected result finds its origin in the resonant behaviour of the optical index of silica in the mid-infrared. On a dimer of patch antennas, the spectral signature of hybrid modes resulting from near-field coupling is observed [4].
Dielectric microspheres are also attractive to tailor the thermal radiation spectrum. For single silica microspheres, we evidence the excitation of both surface phonon-polariton (SPhP) modes and geometrical electric and magnetic Mie modes. The transition from a phonon-mode-dominated to a Mie-mode-dominated emission spectrum is observed [5].

References

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Modeling Radiative Heat Transfer at the Micro/Nanoscale using the Thermal Discrete Dipole Approximation

Sheila Edalatpour

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Radiative heat transfer is said to be in the micro/nanoscale regime when the size of the heat exchanging media or their separation distance is comparable to or smaller than thermal wavelength (approximately 10 μm at room temperature). In this regime, the Planck theory of blackbody thermal radiation and the radiative transfer equation used for describing radiative heat transfer at the macroscale are not valid anymore. Instead, fluctuational electrodynamics is used for describing radiative heat transfer at the micro/nanoscale. At sub-wavelength separation distances, the electromagnetic evanescent waves contribute and dominate radiative heat transfer, and the heat exchange rate exceeds the far-field blackbody limit by several orders of magnitude. When the size of the heat-exchanging media approaches sub-wavelength values, thermal radiative properties of the media are significantly affected, such that radiative heat transfer between sub-wavelength objects can be very different from that for corresponding macroscopic media. For these reasons, radiative heat transfer at the micro/nanoscale scale is very promising for applications such as nano-gap thermophotovoltaic power generation, photonic refrigeration, and designing materials with novel thermal radiative properties.

Most of these applications require modeling radiative heat transfer in complex geometries for which analytical solutions do not exist. Numerical methods such as thermal discrete dipole approximation (T-DDA), boundary element method, finite difference time domain and frequency domain methods, and Fourier modal method (also called rigorous coupled wave analysis) have been developed for modeling radiative heat transfer at the micro/nanoscale. T-DDA is a volume discretization method in which the volume integral form of Maxwell's equations augmented with the thermal stochastic current (the source of thermal radiation) is solved numerically. The T-DDA is a very versatile method, and it can be used for modeling radiative heat transfer in arbitrary geometries, geometries including an infinite surface, as well as periodic geometries. This talk is focused on the T-DDA. The formalism of the T-DDA is presented, and its application to some fundamental and practical problems will be discussed.

Non-Fourier time-harmonic photothermal heating by nanoparticles

R. Esquivel-Sirvent and **A. Camacho de la Rosa**

[1]*Instituto de Física, Universidad Nacional Autónoma de México*
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The time-harmonic heating of a non- Fourier medium by spherical nanoparticles via the photothermal effect is studied. The nanoparticle is embedded in a medium with thermal properties similar to those reported for organic tissue that does not obey Fourier's law of heat conduction but rather the Cattaneo− Vernotte equation. We show that the temperature profile outside the nanoparticle oscillates and, at specific separations, can have a temperature 16% lower than predicted using Fourier's law of heat conduction. Finally, we discuss some fundamental properties of the thermal waves such as their causal response for different models and the corresponding Kramers-Kronig relations for the heat problem.

References

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Non-Reciprocal Thermal Radiation and Energy Harvesting

Shanhui Fan[1], Yubin Park[1], Zunaid Omar[1], Bo Zhao[1], Cheng Guo[1], Viktar S. Asadchy[1], and Jiahui Wang[1]

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We present some of our recent works of non-reciprocal thermal radiation in the context of solar and thermal energy harvesting. In the context of solar energy harvesting, we introduce the idea of a non-reciprocal multijunction solar cell [1,2], which can reach the Landsberg limit for the efficiency of solar energy harvesting. The Landsberg limit represents the ultimate limit of solar energy harvesting and cannot be reached by the use of any reciprocal systems. We also show that non-reciprocity cannot be used to overcome the Shockley-Queisser limit in single junction solar cells [3]. In the context of thermal energy harvesting, we show that the use of non-reciprocity can theoretically lead to photon-based thermal engines that operate at Carnot efficiency limit with non-zero power. And we discuss the connection of non-reciprocal thermal engines [5] to the persistent heat current in non-reciprocal thermal photonic systems [6].

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Quantum Friction near nonreciprocal media

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We investigate how the quantum friction experienced by a polarisable charged particle moving with constant velocity parallel to a planar interface is modified when the latter consists of nonreciprocal media, with special focus on topological insulators. We use macroscopic quantum electrodynamics to obtain the Casimir--Polder frequency shift and decay rate. These results are a generalization of the respective quantities to matter with time-reversal symmetry breaking which violates the Lorentz reciprocity principle. We illustrate our findings by examining the nonretarded and retarded limits for three examples: a perfectly conducting mirror, a perfectly reflecting nonreciprocal mirror and a three-dimensional topological insulator.

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Thermocurrent spectroscopy of Yu-Shiba-Rusinov states in single-molecule junctions

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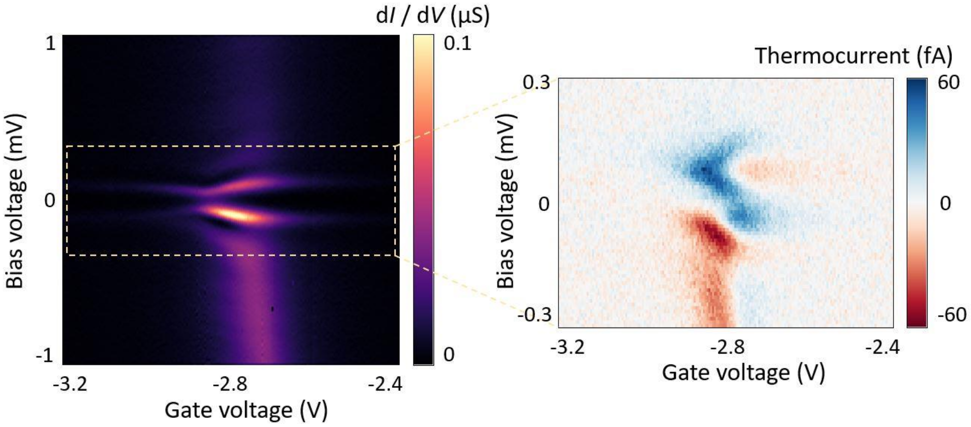
The interaction between magnetic impurities and superconductors leads to fascinating physical phenomena resulting from the competition between Kondo screening and Cooper pair formation [1]. To this end, individual magnetic impurities can form states within the superconducting gap, called Yu-Shiba-Rusinov (YSR) states [1,2]. YSR states are of great interest because they have the potential to realise topological superconductivity. Here we show that such YSR states form in a neutral and stable all-organic radical molecule coupled to proximity induced superconducting break-junction electrodes. We experimentally study the thermoelectric response [3] of the system at mK temperatures, both in the YSR regime and – by applying magnetic fields – in the Kondo regime [4]. Ultimately, we observe a two-fold increase of the thermoelectric efficiency which is induced by the YSR states. This study highlights the power of thermocurrent measurements as a new spectroscopic tool to study nanoscale devices, and reveals new strategies for engineering highly efficient thermoelectric energy conversion at cryogenic temperatures.



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Heat transfer modelling in the crossover regime between conduction and radiation

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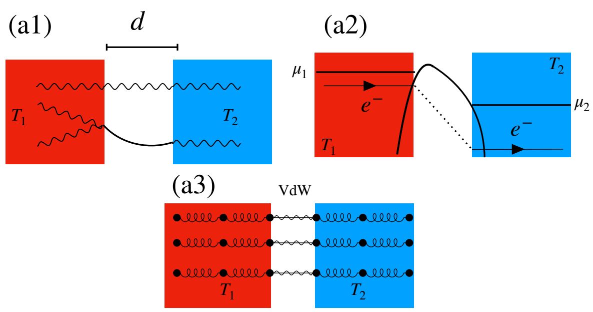
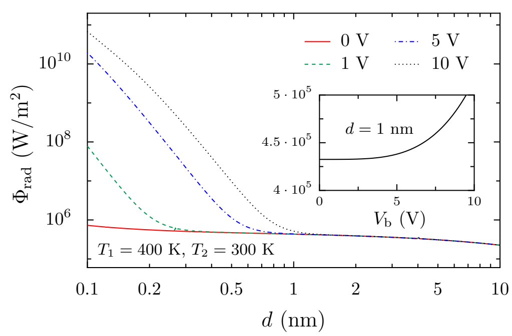


(a) Illustration of the different heat exchange mechanisms between two metals at temperatures T_1 and T_2 and chemical potentials μ_1 and μ_2, respectively, for gap distances $d \leq 1$nm. (a1) Propagative and evanescent electromagnetic radiation (a2) Electron tunneling through electrostatic and image force potentials (a3) Acoustic phonon tunneling due to Van der Waals forces.



(b) Radiative heat flux between two semi-infinite gold slabs with respect to the gap thickness d for different bias voltages. Inset: Radiative heat flux as a function of bias voltage.

In the near field (for separation distances smaller than the thermal wavelength, of the order of some microns at ambient temperature), the radiative heat flow between two solids at different temperatures can exceed the far field limit by several orders of magnitude. At even smaller distances, in the so-called extreme near field (distances in the nanometer range and below) the physics changes radically, since acoustic phonons and electrons can contribute as further channels to the heat exchange [1, 2]. Here we introduce a theoretical framework to describe the heat transfer mediated by these carriers between two metallic bodies. We quantify the role of electron tunnelling currents using semiclassical and fully quantum approaches, by paying attention to the role played by the shape of the electronic barrier. Using an approach based on the elastic theory, we address the role of acoustic phonons coupled through the Van der Waals and the electrostatic forces. Finally, we employ the fluctuational electrodynamics theory to study the role played by photons, by adding the contribution of non-local effects. This theoretical work allows us to assess the relative weight of the different carriers with respect to the separation distance, and to highlight the crucial role played by the external bias voltage on the heat flux carried by the three types of carriers.

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Atomistic simulation of phonon tunneling across metallic vacuum nanogaps

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The understanding of extremely near-field heat transport remains an open question. The two recent experimental reports [1, 2] in this regime have shown controversial results. Kloppstech et al. [1] observed giant thermal conductance whereas Cui et al. [2] found much smaller values below the detection resolution. Phonon tunneling across nanogaps has been put forward as an important mechanism explaining the giant heat transfer observed experimentally.

In this work [3], we present a fully three-dimensional atomistic simulation framework by combining the molecular dynamics (MD) and phonon non-equilibrium Green's function (NEGF) method. The relaxed atomic configuration and interatomic force constants of metallic nanogaps are generated from MD as inputs into harmonic phonon NEGF. Phonon tunneling across gold-gold and copper-copper nanogaps are quantified, and is shown to be a dominant heat transport channel for gap size below 1nm. Through a comparison of the results by MD and NEGF as anharmonic and harmonic approaches respectively, we demonstrate ~20-30% contribution of lattice anharmonicity to phonon tunneling across the nanogap. In addition, the electrostatic interaction turns out to have negligible effect for the small bias voltage typically used in experimental measurements. Our atomistic simulation is consistent with the experiment by Cui et al. [2] while still not able to explain the giant heat transfer in the experiment by Kloppstech et al. [1]. We conclude that phonon tunneling alone can not explain the giant heat transfer seen in the latter experiments.

The present atomistic simulation framework provides a more pertinent modeling of the phonon heat transport channel and hitherto detailed information of the heat current spectrum across metallic nanogaps. Our study contributes to deeper insight into heat transport in the extremely near-field regime, as well as hints for the future experimental investigation.

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Generalized coupled dipole method for thermal far-field radiation

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We introduce a many body theory for thermal far-field emission of dipolar dielectric and metallic nanoparticles close to a substrate within fluctuational electrodynamics [1]. This theory renders it possible to assign distinct temperatures to each nanoparticle, substrate, and background which, for example, is necessary to describe experiments like TRSTM [2], TINS [3], or SNoiM [4]. We exemplary determine the radiation emitted by four separated nanoparticles above a substrate for different material compositions of SiC and Ag in the spirit of [5]. Moreover, we perform discrete dipole approximation to model thermal emission of a SiO2 particle in vacuum and thermal far-field radiation of a Si tip close to a SiC substrate like in [6].

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Thermal rectification in quantum systems.

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We address in this work the question of thermal rectification in quantum systems. We will first recall some results about the way to fabricate a thermal diode with the help of 2 two level systems (TLS) or qubits in interaction, each one being related to a thermostat (Fig. 1) [1]. We will show that rectification appears once one thermostat involved has a typical temperature smaller than the TLS energy interaction or energy gap. We also show that the stronger is the coupling, the stronger are the heat current in the system but the lower is the rectification [2].
In a second part, we show that it is possible to make a thermal transistor with 3 TLS, where each TLS is also related to a thermostat. In such a device, two reservoirs impose their temperatures to two TLS, that, in analogy with an electronic transistor can be considered as the emitter and the collector. The heat flux between these two TLS is controlled by the temperature and the heat flux through a third TLS that can be seen as the base (Fig. 3). Depending on the system parameters, a tiny thermal current variation through the base induces a strong variation of the emitter and collector thermal current: this is the thermal transistor effect [3].
We will see that the type of interaction between is critical in the existence of a thermal transistor effect and on the resilience of the effects in future real device. We will see in particular that in the case of interacting spin in the z direction, a $\sigma_x \sigma_x$ interaction is more robust that a $\sigma_z \sigma_z$ interaction [4].

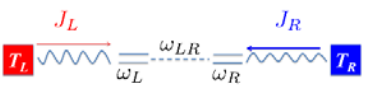

Fig. 1 : Quantum thermal diode scheme made of two spin in interaction

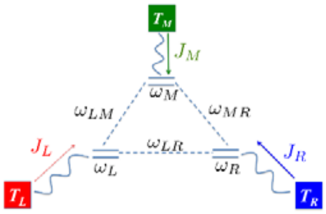

Fig. 2 : Quantum thermal transistor scheme made of three spin in interaction (spin ring model)

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Mesoscopic theory and phenomena of fluctuational electrodynamics

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The fluctuating electromagnetic field leads to a variety of mesoscopic phenomena, including the famous Casimir or van der Waals effects. Recent interest and work has gone far beyond these original considerations in many aspects, for example, by including non-equilibrium scenarios, investigation of nanoscopic geometries, or by studying modern materials, both in theory as well as in experiments.

In this contribution, I will introduce scattering theory as a tool for analysis and investigation of phenomena induced by the fluctuating electromagnetic field in the mentioned situations. Specific examples include recent work on fluctuation induced forces acting between non-reciprocal media for setups in and out of equilibrium [1] [2].

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Solid-state pyroelectric system for near-field energy conversion

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We introduce [1] a mechanism to convert near-field energy using micrometric pyroelectric membranes encapsulated between two graphene field-effect transistors [2] which act as the hot source and cold sink. By modulating the gate voltage in the graphene transistors, the radiative coupling between the pyroelectric membrane and both the source and the sink can be modulated as well. This dynamical modulation can induce controlled temperature variations in the active layer, so useful energy can be obtained thanks to the pyroelectric properties of the layer. We show with an example that these systems can generate a power of 130 mW/cm2 using pyroelectric Ericsson cycles, a value which surpasses the current production capacity of near-field thermophotovoltaic conversion devices [3-5] with low-grade heat sources ($T < 500$ K) and small temperature differences ($\Delta T \sim 100$ K). The temperature of the active layer can be modulated at kHz frequencies with the proposed solid-state device, achieving power densities higher than those obtained with mechanical pyroelectric converters [6]. We also show that our graphene-based pyroelectric system is a self-powered conversion device in which the power required to modulate the temperature is much smaller than the delivered power, opening so a new avenue for high-frequency pyroelectric energy harvesting from stationary thermal sources.

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Near-Field Thermal Radiation and Photovoltaic Energy Conversion

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Near-field thermal radiation occurs when two objects are located closer than the characteristic wavelength of thermal radiation determined by Wien's displacement law. At such small vacuum gap distances, the radiative heat transfer can exceed the blackbody radiation limit due to photon tunneling of evanescent waves. Despite abundant theoretical works, experimental demonstration of the near-field thermal radiation between flat surfaces is rather limited because of great challenges in maintaining a nanogap between planar surfaces with a large surface area. This presentation will give an overview of our endeavor on quantitative measurements of the near-field thermal radiation between doped-Si plates [1], Ti/MgF_2 metallo-dielectric multilayers [2], and thin Ti films [3]. Finally, our recent work about near-field thermophotovoltaic energy conversion [4] will be introduced.

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Convection-type heat transfer behavior in the asymmetric nanoparticle chains via thermal photons

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Near-field radiative heat transfer (NFRHT) in nanostructure networks recently attracts a lot of research interests. When separation between nanostructures is comparable to or less than the characteristic thermal wavelength, the near-field effects become important and the radiative heat flux can exceed the Planckian blackbody limit by several orders of magnitudes. In the nanoparticle networks, nanoparticles usually lie in the near field of each other, which results in the significant multiple scattering of the thermally excited electromagnetic waves, namely many-body interaction (MBI). The complex MBI significantly affects the heat transfer behavior inside nanoparticle networks. The heat superdiffusion was proved in the ordered chain with strong MBI. However, few results on heat transfer in asymmetric chains have ever been reported, due to lack of well-developed continuum-scale theoretical framework before. Our recent work provides a normal-diffusion theory from fluctuational electrodynamics for asymmetric structures. In this work, heat transfer in asymmetric nanoparticle chains is investigated by means of the normal-diffusion theory [1]. Effect of the asymmetry of structure on NFRHT is analyzed. The spatial distributions (profiles) of temperature and heat transfer coefficients (i.e., the effective thermal conductivity [ETC] and the asymmetrical photonic heat transfer coefficient [APHTC]) along the chain are also analyzed. For heat transfer in asymmetric nanoparticle chains via thermal photons, in addition to the heat diffusion process, the convection-type heat transfer process caused by the asymmetry of the structure also exists. Heat transfer in the asymmetric chain has an obvious preferential direction, which is due to the existence of the convection-type heat transfer process via thermal photons. In the considered asymmetric nanoparticle chains, the spatial variation of nanoparticle packed density is obvious, which results in the spatial-dependent heat transfer coefficients. Magnitude of both ETC and APHTC for the position with densely packed nanoparticles is much larger than that of the position with loosely packed nanoparticles. The sign of APHTC means for the preferential direction of heat transfer. For the asymmetric chain where nanoparticles pack densely at the left hand side and packs loosely at the right hand side, the sign of the APHTC is '-' meaning for the heat transfer preferential direction from left to right. It is also noted that temperature gradient along the asymmetric chain varies from position to position and increases with decreasing the effective thermal conductivity.

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Recent progress in the theory of acoustic phonon tunneling across a vacuum gap between piezoelectric crystals

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It is known from the literature that an acoustic wave can “jump” or “tunnel” across a vacuum gap between two piezoelectric solids. However, the cases studied before have been particularly simple examples, and a more general approach has not been formulated. Recently, we remedied that situation, by presenting a more general formalism and approach to study such a phonon tunneling effect between two arbitrarily oriented anisotropic piezoelectric semi-infinite crystals (plane-plane geometry) [1]. The approach allows one to solve for the reflection and transmission coefficients of all the partial-wave modes, and is amenable to practical numerical, or in some cases analytical implementation.

Within the formalism at hand, we have discovered that complete tunneling, i.e. transmission with probability one, is possible for a large range of crystal orientations. We discuss a simple resonance condition that has to be satisfied to allow for the complete tunneling effect to happen and write it in terms of the effective electrical surface permittivity of the piezoelectric crystal [2].

Finally, we present results of the application of our theory to heat transfer across a nanoscale vacuum gap, showing that (i) the rotation of the crystal can be used to modulate the heat flux by about an order of magnitude, and that (ii) acoustic phonon tunneling can dominate over all other near-field mechanisms at low temperatures below 100 K for nanoscale gaps.

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Phonon transport at interfaces: from Kapitza resistance to single molecule junctions

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Understanding and predicting the behavior of phonon at interfaces is of a great importance for microelectronics where thermal management is a vital issue [1,2]. Maximizing heat removal at interfaces is critical to avoid hot spots and thermal throttling in modern computers and 5G smartphones.

In this tutorial, we will start by introducing briefly the physics of phonons in the bulk and at interfaces. We will also devote some time to present the different computational techniques which allow one to study interfacial thermal transfer, namely lattice dynamics, molecular dynamics and non-equilibrium Green's functions [3,4]. We should discuss to which extent the computational models compare to experimental investigations. In particular, the role of electron-phonon processes at the interfaces will be discussed [5].

In the second part of the talk, we will illustrate how atomistic calculations may help understand the physics of extreme near field heat transfer [6]. Among other topics, we will discuss phonon transport across molecular junctions [7]. We propose different strategies to enhance their thermoelectric efficiencies based on the consideration of different pending groups and molecular bridges [7].

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Coupling between conduction and near-field radiative heat transfer in tip-plane geometry

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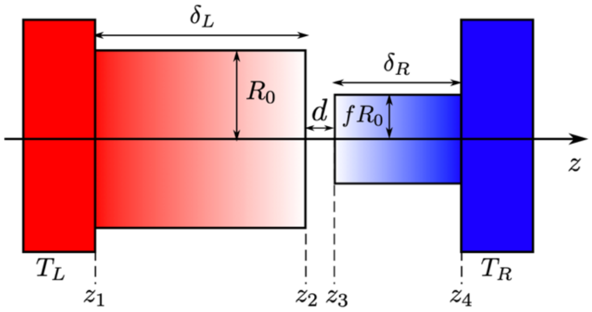
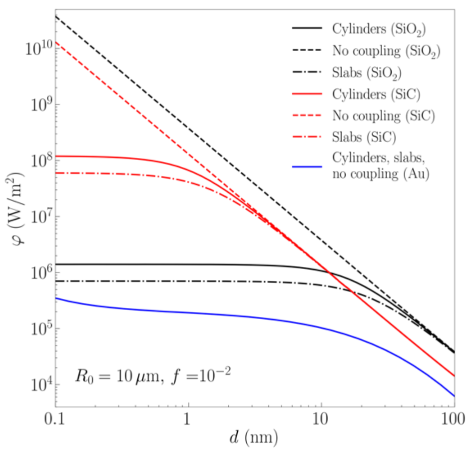
The radiative heat flux between two bodies, limited at large distance by Stefan-Boltzmann's law, can dramatically increase in the near field because of photon tunneling. Although this prediction has been confirmed in many experiments, some of them have observed deviations from theoretical results, both in near field [1] and in extreme near field [2,3]. In this sense, one possibly relevant aspect could be is the coupling between exchanged radiative flux and conduction. For two parallel slabs, this coupling [4,5] was shown to can induce a temperature profile in each body and a saturation of the exchanged flux. In this work [6] we consider two concentric cylinders of different radii, allowing us to simulate the configuration of a sharp tip in front of a plane. We obtain expressions for both the temperature profiles and the exchanged flux, showing that also in this scenario the conduction-radiation coupling can induce a significant temperature change in the smaller cylinder (the tip), up to tens of degrees in the case of polar materials, along with a strong reduction of the flux (of more than two orders of magnitude) with respect to the scenario of absence of coupling.





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Effect of superconducting transition on near field heat transfer

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We present results of experiments motivated by demands on reduction of radiative heat transfer (RHT) in low temperature devices. We studied radiative heat transfer between metallic materials both in far field (FF] [1] and in field of thermal evanescent waves, in the so called near field (NF) [2, 3], including the effect of the superconducting (SC) transition on RHT in low critical temperature superconductors (LTS) [4, 5]. At room temperatures and lower, the RHT between metals is dominantly mediated by free electrons. Hence a question of what happens when electrons of LTS condense in Cooper pairs and SC energy gap opens below critical temperature Tc of transition to superconductivity. While the effect of transition to superconducting state on FF RHT is weak, the effect in NF is strong. Surprisingly, the contrast between NF RHT in normal and SC states remains sizable even at high temperatures of the hot sample (radiator) with the characteristic energy of radiation far above the SC energy gap. Experimental results of SC effect are interpreted using the Polder [6] relations for RHT, the measured electrical dc resistivity applied to computer code [7] for calculation of dynamical electrical conductivity derived from Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity [8] and the calculated Fresnel coefficients for a sample consisting of a metallic layer on sapphire substrate. This way, we can explain the limits on RHT suppression in the SC state due to different behaviours of transversal electric and magnetic radiation modes. Due to the suppression of NF in superconducting state, we could observe a weak effect of destructive interference of thermal radiation near the FF to NF RHT transition. Considering the strong effects of SC on the NF RHT in the metallic superconductors, which are low temperature superconductors (LTS) showing low transition temperature Tc, it is interesting to consider NF RHT in high-T_c superconductors (HTS). In the last part of the talk, we discuss the possible effects on RHT of HTS, namely YbaCuO (T_c about 90K), on the basis of optical properties [9] and the published calculated NF RHT in HTS [10].

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Thermal conductance
of single-atom and single-molecule junctions

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Single-atom and single-molecule junctions turn out to be ideal platforms for testing quantum theories that are required to describe charge and energy transport in novel nanoscale devices. Until recently, however, the thermal conductance of single-atom and single-molecule junctions has not been experimentally accessible, owing to the challenge of detecting minute heat currents at the picowatt level. In this presentation, I will discuss how picowatt-resolution scanning probes, previously developed to study the thermal conductance of metallic single-atom junctions [1-3], allow to measure the thermal conductance of single-molecule junctions [4]. At the example of single-atom and single-molecule junctions, I will discuss our present theoretical understanding of heat transport at the atomic scale based on first principles and molecular dynamics computational modeling [4-7].

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Energy Transfer and Conversion in Nanoscale Gaps

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Understanding radiative heat transfer in nanoscale gaps and devices is of considerable interest for creating novel energy conversion devices. In this talk, I will first describe ongoing efforts in our group to experimentally elucidate nanoscale radiative heat transfer. I will present our recent experimental work where we have explored how radiative heat transfer is modified in nanoscale gaps at room temperature and cryogenic temperatures. Specifically, I will describe a variety of instrumentation including novel nanopositioning platforms and microdevices, which we have developed to accomplish these measurements. Further, I will discuss possible applications of near-field thermal radiation for energy conversion and photonic cooling. Finally, I will briefly outline how these technical advances can be leveraged for future investigations of nanoscale heat transport and near-field thermophotovoltaic energy conversion.

Limits on light–matter coupling at the nanoscale

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We survey a recently proposed framework based on the mathematics of Lagrange duality that enables calculation of a wide range of electromagnetic limits. The technique establishes physical bounds as quadratically constrained quadratic programs that, while relaxing the requirements of local wave physics contained in Maxwell's equations, incorporate as a set of spatial constraints on otherwise free wave objectives, the imposition of energy conservation at various length scales. We showcase the generality and utility of this framework by discussing recent limits on thermal emission, radiative heat transfer, and more generally the electromagnetic response of sources in nanostructured environments. As shown, the resulting scaling laws and bound quantities illustrate key features related to the possible yet limited ways through which materials and geometry may be used to enhance light–matter coupling and energy propagation at the nanoscale. Radiative heat transfer between two bodies may be enhanced in the near field but is limited by the degree to which multiple scattering between bodies may be controlled. Relatedly, Purcell enhancement or the local electromagnetic density of state increases rapidly in the vicinity of structured medium but is highly constrained by spectral sum rules, saturating in proportion to the bandwidth even in the limit of infinite material response. Beyond scaling laws, the bounds provide quantitative guidance for the expected performance of nanostructured materials in enhancing a variety of light–matter objectives, coming within factors of unity from high-performing devices—sophisticated versions of gratings, bowtie antennas, and resonators—obtained through the machinery of large-scale optimization or inverse design.

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Extended Förster's theory to include dynamic effects in resonance energy transfer

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Non-radiative dipole-dipole interactions are responsible for several important phenomena including near-field heat transfer and resonance energy transfer. Here, by considering the dipole-dipole interactions between two level systems we attempt to model the resonance energy transfer between two molecules beyond the weak perturbation limit. The goal of this work is to see if the dynamics of energy transfer between two molecules can be reasonably captured by a simple technique of utilizing the well-known text book result of population dynamics of a two-level system along with the knowledge of experimentally obtained fluorescent and absorption spectra of the molecules. We compare our results with exact simulation results from hierarchical equations of motion technique present in literature. We also show that, for certain cases, it is possible to derive a time-dependent Förster's rate-like expression for the rate of energy transfer in the weak-coupling regime.

Nonmonotonous Temperature Dependence of the Thermopower of Gold Atomic Contacts

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Understanding the interplay between electronic and phononic transport in nanoscale conductors is of fundamental interest and important for the development of functional devices, in particular for those combining charge and heat transport. The charge and heat transport down to the ultimate small size scale of few-atom contacts is meanwhile well understood, in particular in the quantum coherent regime that is covered by the Landauer theory.

Single-atom gold atomic contacts are considered as archetypical quantum coherent conductors since they show an almost perfect quantization for the conductance to G = 1 G_0 (with the conductance quantum $G_0 = 2e^2/h$).

Also the Seebeck coefficient which describes the thermopower of atomic gold contacts has been studied by different methods at room temperature and at low temperature, however using different realizations of the contacts. At low temperature the Seebeck coefficient vanishes in agreement with theory, while at room temperature it adopts a small negative value.

We now performed measurements of the thermopower of atomic-size gold contacts realized by the mechanically controllable break junction (MCBJ) technique over a temperature range from ~10 K to 295 K. While the conductance histograms confirm the quantum nature of the transport, we observe a non-monotonous temperature dependence of the ensemble-averaged thermopower with a minimum of -2 µV/K at about 150 K. Our observations at low and high temperature are compatible with values reported in the literature, but the non-monotonous behavior in between disagrees with the expected linear increase of the thermopower for quantum coherent conductors described by the Landauer formula.

We discuss several possible mechanisms that may be at the origin of the deviation, including of phonon contributions to the thermopower, as well as slight deviations from a constant transmission function. Our findings show that, firstly, the thermopower gives important insight into the transport properties of atomic-size structures and second that the linear approximation of the Landauer model has to be used with caution when studying more complex transport properties.

Theory of electronic noise and simulations of phonon transport in molecular-scale junctions

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I will divide my talk to two parts beginning with studies of electronic noise in nanojunctions using a quantum coherent theory and finishing in the opposite side, with our simulations of phonon conduction using classical methods. First, I will focus on charge carriers and describe our recent theoretical studies of new (and old) noise contributions in atomic scale junctions, in collaboration with an experimental group. Here, I will give you a survey of different noise components that we had studied or discovered, including shot noise activated by voltage bias or a temperature difference [1], and the flicker noise arising from fluctuating defects [2]. Our main question in these explorations has been what new information on quantum transport one can extract from charge current fluctuations. In the second part, I will talk about our interest in phonon transport through molecular junctions [3]. Here, I will describe simulations using classical molecular dynamics techniques [4]. After explaining the methodology and benchmarking, I will tell you about our efforts and challenges in creating a molecular-level thermal diode device.

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Electron-phonon coupling in metals under ultrashort laser irradiation: two-temperature model

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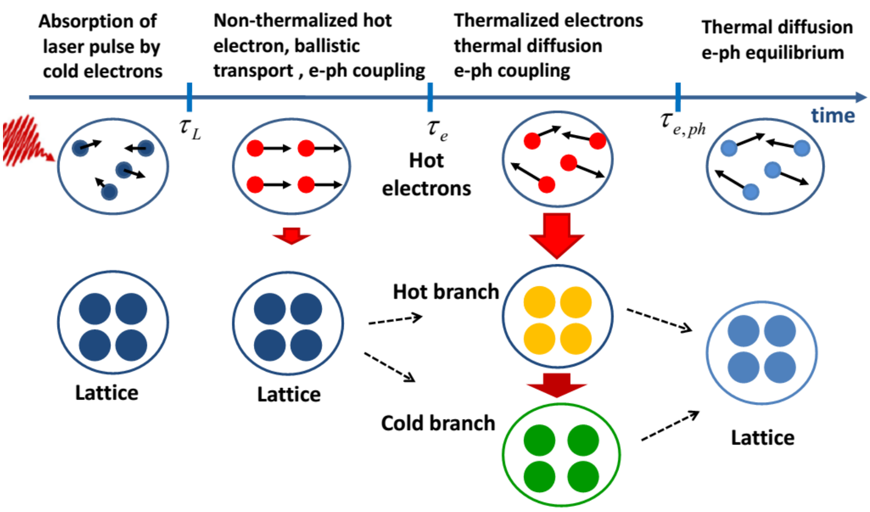
The coupling between different excitations in complex nanosized systems leads to the multiple time and space scales nature of out-of-equilibrium thermal dynamics, which is manifested by the non-Fourier effects, such as multi-front wave-like temperature propagation and boundary temperature jumps. The dynamics is described by a hierarchy of partial differential equations of high order with a series of consecutive relaxation times characterizing different modes. The fastest mode is the relaxation of nonequilibrium energy carriers to local equilibrium, which represents a wave-like propagation of temperature discontinuity. The fastest front is followed by continuous wave-like structures due to successive couplings between different excitations. The fronts can be experimentally detected at times that are long relative to the relaxation time of the fastest mode but short on the time scales characterizing the relaxation of the system to equilibrium. The TTM approach seems to be universal and can be used to study the coupling effects in complex nanosized systems, such as metals, heterogeneous systems, metamaterials like layered correlated materials, nanosized graphene, bio-heat systems, where coupling between different excitations play a significant role.



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Thermal transport in twisted 2D materials

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Varying the angle between two or more 2D material layers drastically affects the physical properties of the stack. Indeed, in such twisted systems, the atomic reconstruction leads to the formation of a Moiré pattern and thus breaking the lattice symmetry. By varying the rotational misalignment between the layers and controlling the twist angle, it is possible to engineer the stack properties and unravel unexpected phenomena. While electronic transport has been extensively studied in twisted bilayer graphene, thermal and thermoelectrical properties remain largely to be explored - minute experimental results have been published on the subject. In this work, we report the direct observation of thermal transport in twisted double bilayer graphene (TDBG) rotated by a small angle (<1°) using high vacuum Scanning Thermal Microscopy (SThM). The sample was fabricated by stacking on hexagonal boron nitride two graphene bilayers at a tiny angle to create large Moiré cells. We first confirmed the presence of lattice reconstructed areas and the effective twist angle using Piezoresponse Force Microscopy. Then, we turned to in situ thermal transport imaging of those regions. SThM measurements allowed to locally observe and quantify a thermal resistance increase of the twisted area compared to Bernal stacked layers. Our results are in lign with several theoretical and computational reports for similar systems. This study paves the way for numerous thermal transport experiments in twisted 2D materials systems.

Surface Phonon-Polaritons as Efficient Heat Carriers

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Recent studies showed that surface phonon-polaritons, i.e. evanescent electromagnetic waves propagating along the surface of polar dielectric materials [1] [2], may potentially serve as novel heat carriers to enhance the thermal performance in micro- and nanoscale devices.
This seminar will expose the significant contribution of these carriers to thermal conductivity in ultra-thin (<100nm) films [3], but also to radiation, yielding SuperPlanckian emission and absorption between surfaces of larger scales (10mm).

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Dependent scattering in thick and concentrated colloidal suspensions

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Radiation transfer through colloidal suspensions has been modeled with the radiative transfer equation (RTE) assuming independent scattering. Then, the effective absorption and scattering coefficients of the dispersed medium are predicted based on superposition principle. However, this approach is not valid when the interparticle distance is on the same order of magnitude as the wavelength corresponding to when the volume fraction is large. This situation is referred to as dependent scattering. Then, the radiation characteristics of the ensemble of particles needs to be predicted by solving Maxwell's equations. Here we use the radiative transfer with reciprocal transactions method (R^2T^2) to predict the transmittance of plane-parallel slabs of suspensions while accounting for dependent scattering effects. A wide range of particle size parameters, and particle volume fraction were investigated. Dependent scattering effects were found to prevail for particle volume fraction higher than 2% depending on the particle size. Evidence of dependent scattering was also observed experimentally in the visible transmittance of colloidal suspensions of silica nanoparticles with average diameter of ~20 nm and particle volume fraction ranging from 2% to 15%. Good agreement was found between experimental measurements and numerical predictions accounting for dependent scattering. The transmittance decreased with increasing particle volume fraction but dependent scattering limited that decay compared with solutions of the RTE assuming independent scattering. Later we extended the method to agglomerated structures and we observed the R^2T^2 could solve the light transfer through the porous mediums rigorously.

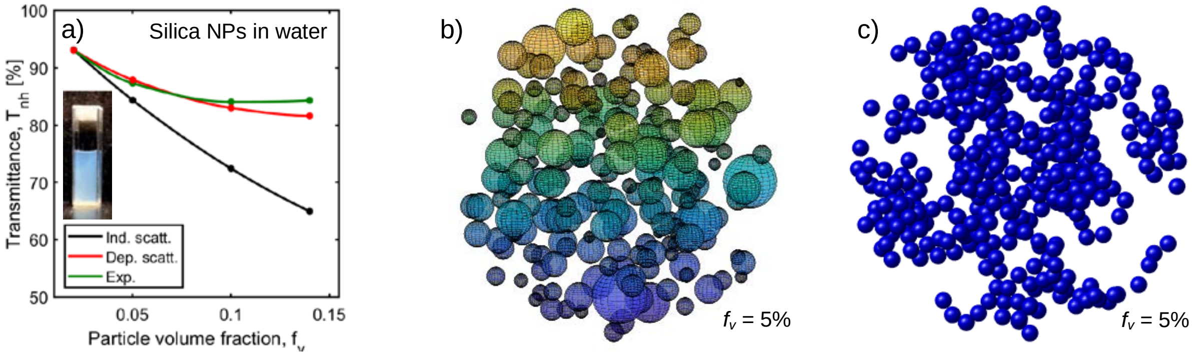

Figure 1. (a) Comparison of the spectral normal-hemispherical transmittance $T_{nh,\lambda}$ measured experimentally and predicted by the R^2T^2 method accounting for dependent scattering and the classical Monte Carlo method assuming independent scattering at 500 nm for L = 10 mm. Example of computationally generated ensembles of (b) randomly distributed and (c) aggregated structures.

SQUID-on-tip nanoscale thermal imaging: Glimpse into dissipation in quantum systems down to atomic scale

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Energy dissipation is a fundamental process governing the dynamics of classical and quantum systems. Despite its vital importance, direct imaging and microscopy of dissipation in quantum systems is currently very challenging. We have developed a scanning nanoSQUID that resides at the apex of a sharp pipette acting simultaneously as a nanomagnetometer with single spin sensitivity and as a nanothermometer providing cryogenic thermal imaging with 1 μK resolution [1]. The non-contact non-invasive thermometry enables direct visualization and control of the minute heat generated by electrons scattering off a single atomic defect in graphene [2]. By further combining the scanning nanothermometry with simultaneous scanning gate microscopy we demonstrate independent imaging of work and dissipation, reveal the microscopic mechanisms that conceal the true topological protection in the quantum Hall state in graphene [3], and observe long-range dissipation and nontopological edge currents in charge-neutral graphene [4].

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Abstracts of Posters

(in alphabetical order)

CuO/TiO_2 nanocomposite photoanode for dye sensitized solar cell

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Abstract

Dye sensitized solar cells (DSSCs) are preferable as simple and low cost renewable energy technique. In DSSCs the photo-anodes play significant role for collecting and transfer of photo-excited electrons from dye to external electric circuit. The performances of the photo-anode depend on the band gap, morphology and composition. The present work was focused on enhancing the light-harvesting properties of the photo-anodes TiO_2, CuO/TiO_2 nano-composite which is considering a promising way to encourage the efficiency (η) of dye-sensitized solar cells (DSSCs). First, titanium dioxide TiO_2 nanoparticles prepared by hydrothermal methods. The hydrothermal method was used Titanium bis (ammonium lactato) dihydroxide as precursor. XRD showed TiO_2 crystalline anatase phase directly. From the UV-VIS results the absorption spectrum was clear in the UV region there is no absorption in VIS region appeared. The particle size and the morphology were obtained from the HRTEM results. These results indicate that the hydrothermal method is simple and fast way to synthesis of TiO_2 crystalline anatase phase. Second the CuO/TiO_2 nanocomposite was synthesized. The XRD appeared monoclinic structure of CuO and anatase TiO_2 as composite structure. UV-ViS results show there an improvement in the TiO_2 absorption spectrum after introducing of CuO as composite. The HRTEM confirmed that the formation of CuO/TiO_2 nano-composite. The third steps were applied the TiO_2 and CuO/TiO_2 each as photo-anode for dye sensitized solar cell and the efficiency calculated. The DSSC was synthesized by doctor blade method, one of the widely used techniques for producing thin films. Current–voltage measurements (I-V) showed the efficiency achieved by CuO/TiO_2 was higher than the Pure TiO_2 DSSCs.

Radiative cooling of solar cells: detailed opto-electro-thermal modeling and influence of surface structuring

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Silicon solar cells are designed to efficiently absorb solar photons but convert only a limited proportion of the incoming energy into electricity. In real operating conditions, the cells therefore operate at much higher temperatures than in standard test conditions [1]. This heating is detrimental to their energy conversion efficiency and lifetime. Several cooling strategies are therefore being studied to reduce the cell temperature [2]. In recent years, there has been a growing interest in the so-called radiative sky cooling (RSC) strategy. This approach consists in optimising the thermal radiation of cells or modules by taking advantage of the atmospheric transparency in the 8-13 µm range [3]. Although some preliminary studies on the topic predict cooling of more than 13 °C on silicon wafers [4], they remain insufficient to fully assess the potential of this technique for various technologies.

In this work, we first give the big picture of radiative sky cooling and discuss some peculiarities when applied to photovoltaic devices. Using a fundamental modelling framework developed during the thesis [5], we then show the great benefit of enhanced RSC. Furthermore, we unveil the ideal thermal emissivity profile needed to achieve the best cooling performance. In a second step, we make a focus on photonic improvement pathways. Using a transfer matrix method, we simulate the thermal emissivity of a silicon module from the visible to the mid-infrared range. This allows us to investigate practical pathways for improved RSC.

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Localized edge states in radiative heat transfer

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Many efforts have been dedicated to manipulate the radiative heat transfer by designing different kinds of geometrical morphology or introducing artificial materials [1-3]. Various unusual behavior of artificial materials is governed by their topological properties, among which the edge state in photonic crystals has been captivated as a popular notation. The Su–Schrieffer–Heeger (SSH) model, which is a simple lattice configuration that exhibits topological edge states, has been widely used for investigating topological modes in various physical branches [4-6]. Inspired by the SSH model, we have explored the topological aspect of the radiative heat transfer in a given array of nanoparticles. We demonstrate the existence of bulk-boundary correspondence and localized edge states in radiative heat transfer seeking new aspects to prior works such as heat flux in a coexistent double chain of trivial and non-trivial states.

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Mechanisms to Tailor the Phononic Thermal Conductance of Molecular Junctions Unveiled by a Genetic Algorithm

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Measurements of the thermal conductance of single molecules have recently been reported for the first time [1,2]. These experiments may found the new field of "molecular phononics", where single molecules are used to tailor the phononic thermal conductance. However, the search for molecules with low or high thermal conductance is complicated by the huge chemical space. Presently, few mechanisms are known to suppress the phononic thermal conductance. Here we describe a systematic search for molecules with a low thermal conductance using a genetic algorithm. Beyond structures of well performing molecules, delivered by the genetic algorithm, we analyze patterns and identify different new mechanisms to suppress phonon heat flow. The identified mechanisms are systematically analyzed on different levels of theory and their significance is classified. Our findings may be of great importance for the emerging field of molecular phononics.

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Crystalline silicon based suspeded thermometry platforms: study of quantum phononic effects

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In this work we aim at learning more about the different thermal transport regimes and the phonon behaviour at very low temperatures (down to several mk) in nanoscale materials. In these conditions, the mean free path Λ and dominant wavelength λ_{DOM} of phonons become equal or greater than the size of a sample, giving rise to several interesting phenomena: phonon interferometric effects [1], thermal rectification behaviour, quantization of thermal transport [2], etc... The project is done in collaboration with CEA-LITEN (Grenoble) for theoretical simulations and with Institut Néel (Grenoble) for sample fabrication and low temperature measurements.

Our fabrication process is based on suspended thermal sensor platforms [3][4]. Institut Néel's team has history on amorphous silicon nitride devices with a two thermal reservoirs design, but at the IEMN we will adapt the fabrication process to a crystalline silicon technology. The devices will be produced from silicon-on-insulator (SOI) wafer by means of top-down micro-/nano-fabrication techniques. Each thermal reservoir has a metallic heater and a thermometer. The sensing will be done by use of the precise superconducting NbN material, and we hope to achieve sensitivities up to zeptowatts (10^{-21} W). Different kind of samples will be fabricated in between the sensing platform (nanowires, patterned membranes, etc…). With this poster we will be presenting the scientific and technological challenges associated with the work and the latest results in terms of device fabrication.

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Phonon hydrodynamic transport in 2D materials

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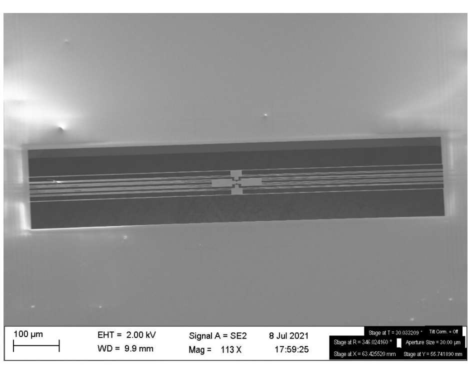
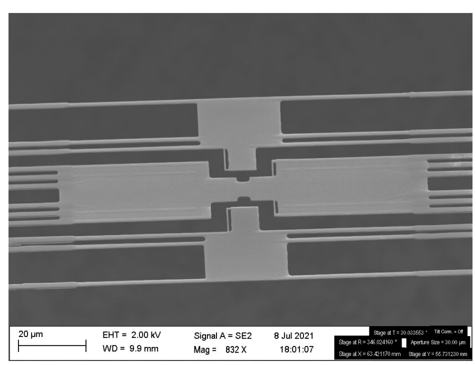
The increasing demand for effective thermal management of microelectronic devices and efficient thermoelectrics has raised the need for new materials with extremely high and exceedingly low, respectively, thermal conductivity. A new phenomenon of heat transport that resemble wave propagation in liquids emerged, known as heat hydrodynamics. This effect arises when normal phonon scattering dominates over Umklapp scattering, thus implying that the phonon momentum is mainly conserved. Probing a deviation of heat flow from diffusive transport requires sensitive thermometers and good thermal isolation from the environment. To this end, a suspended four-terminal device is fabricated, with resistive Joule heaters/thermometer meanders placed on top of underetched silicon nitride (SiNx) membranes. It hangs the sample away from the environment while assessing its thermal conductivity. Furthermore, the device is designed to enable local thermometry using Raman spectroscopy.
Four meanders made of platinum are placed on top of SiNx membranes, which are connected to the substrate by SiNx beams. One meander is electrically heated to generate a heat pulse that raises the temperature on a side of the sample. The remaining thermometers can be used as sensors to probe changes in temperature. A SiNx layer is deposited on both sides of a 2-inch wafer. On one side an etching mask is patterned using direct laser lithography, then through reactive ion etching (RIE) the SiNx is removed, opening windows for the first Si wet etching. The first wet etching is performed using sodium hydroxide (NaOH) and potassium hydroxyde (KOH) so that, a fine mesh of 19 μm squares is etched to partially remove silicon under the devices. On the other side, a photoresist mask is patterned through direct laser lithography to deposit the gold metal contacts for electronic characterization, followed by lift off in DMSO (Dimethyl sulfoxide) to remove the exceeding metal. Using the markers created in the previous step, the gold contacts are aligned with the sites where the devices will be suspended. PMMA photoresist is laid on top of gold to perform an electron beam lithography (EBL), to define the thermometers on top of the membranes through platinum evaporation and lift off. At this point another direct laser lithography step, to outline the suspended SiNx beams of the membranes, is performed and the sample to investigate (Graphene, hBN, others 2D materials) is transferred onto the membranes. Finally, Si wet etching using KOH is done to complete the suspension of the device. Once the fabrication is completed, the sample can be assessed by Raman spectroscopy to map the temperature distribution of the flakes, so that the thermal conductivty is extracted. Currently, we are working on the final step of sample suspension, and once the process is optimazed, the characterization of hBN-Graphene-hBN stack will be performed.





Suspended thermometer, four terminal device. On the left, there is a wide view of the device, the bridged membranes with beams are visible. On the right, there are four suspended membranes of SiNx with the platinum meanders on top, the two central membranes are connected to each other, while the other two side membranes are suspended individually by the beams. This is a scanning electron micrograph acquisition made in the laboratories of University of Basel.

Heat transfer across vacuum gap by piezoelectric acoustic phonon tunneling

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Heat transfer across a vacuum gap is commonly thought to be possible only via far/near field radiation. However, acoustic phonons can also ‘jump’ or ‘tunnel’ through the gap, carrying heat with the help of piezoelectricity. Here we present a theory that can be applied to arbitrarily anisotropic and oriented crystals for such heat transfer mechanism [1]. We found that certain acoustic wave modes can achieve unity transmission for a range of crystal orientations through resonant tunneling. The phonon heat flux between closely spaced solids scales with gap width as d^{-3}, more slowly than other acoustic tunneling mechanisms such as the van der Waals force and the electrostatic potential difference [2,3]. At low temperatures piezoelectricity driven acoustic phonon tunneling can dominate the heat transfer over all other channels, including the near-field EM radiation.

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A New Sensor Concept for Scanning Thermal Microscopy

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Near-field mediated heat transfer (NFMHT) between two surfaces separated by a vacuum gap has become a widely investigated topic in the past decades. To measure this phenomenon, we are using a self-developed near-field scanning thermal microscope (NSThM) based on an STM. It is equipped with self-made thermocouple tips consisting of a platinum wire molten into a borosilicate glass capillary which is then coated with gold. Since the gold layer can also be used as a tunneling electrode, we are able to measure the thermoelectric voltage and the tunneling current between the tip and sample simultaneously. However, the voltage drop due to the tunneling current interferes with the thermo voltage, making break junction experiments investigating heat and electrical conduction uninterpretable. In a new design of the tips for the NSThM, the thermocouple is covered first by an insulating silicon dioxide film and finally by a second gold film, which then acts as a tunneling electrode separate from the thermocouple and eliminates crosstalk. These tips are called PASA-tips due to the sequence of materials (platinum-gold-silicon dioxide-gold). Some example measurements of radiative heat transfer and heat conduction with these tips are shown to illustrate their capabilities.

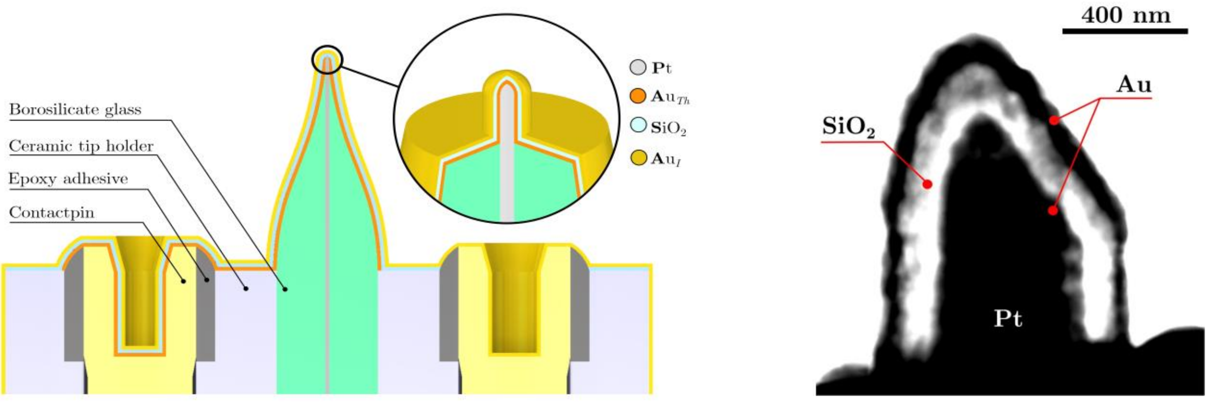

Figure 1: Structure and TEM image of a PASA-tip

Nonthermal Photoinduced Phase Transition

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The underlying innovative concept is that phase transitions, described by the (Helmholtz) free energy *F* are mainly governed by thermodynamic extensive quantities like (binding) energy and entropy, and by further terms like the sored magneto-static or electro-static energies, or volume, strain energy or surface contributions, or intensive quantities as e.g., pressure or temperature. Electromagnetic fields respectively photons do not enter this balance. V. Ginzburg came up with the idea that the binding energy can efficiently (and extremely fast) be varied by modifying the band structure through electron phonon coupling, which depends on the number of electrons, as well as the number of phonons. The number of phonons can hardly be influenced, if then, either by temperature, or by external vibrations, however the number of electrons in a semiconductor can be modified through photon absorption. Because the binding energy depends on the number of free electrons $N(E_{el})$ in the valence and conduction band, as well as on the band gap, a nonthermal modification of $N(E_{el})$ can trigger a phase transition.

To model the photo-induced phase transition in mathematical detail, we use the Hamiltonian suggested by Kristoffel et al. [2]:

$$\hat{H} = \underbrace{\sum_{\vec{q}j}\left(\frac{1}{2M_j}P_{\vec{q}j}P_{-\vec{q}j} + \frac{M_j}{2}\omega_{\vec{q}j}x_{\vec{q}j}x_{-\vec{q}j}\right) + \sum_{\vec{q}_1 j_1}\sum_{\vec{q}_2 j_2}\sum_{\vec{q}_3 j_3}\sum_{\vec{q}_4 j_4} B(\vec{q}_1 j_1, \vec{q}_2 j_2, \vec{q}_3 j_3, \vec{q}_4 j_4)\, x_{\vec{q}_1 j_1} x_{\vec{q}_2 j_2} x_{\vec{q}_3 j_3} x_{\vec{q}_4 j_4} + \hat{H}_{\mathrm{hI}}}_{\hat{H}_{\mathrm{p}}}$$

$$+ \underbrace{\sum_{\sigma,\vec{k}} \varepsilon_\sigma(\vec{k})\hat{a}^\dagger_{\sigma\vec{k}}\hat{a}_{\sigma\vec{k}} + \hat{H}_{\mathrm{e\text{-}e}}}_{\hat{H}_{\mathrm{e}}} + \underbrace{\frac{1}{\sqrt{N}}\sum_{\sigma\sigma'}\sum_{\vec{k},\vec{k}'}\sum_{\vec{q}j} V^j_{\sigma\sigma'}\left(\vec{q},\vec{k},\vec{k}'\right)\hat{a}^\dagger_{\sigma\vec{k}}\hat{a}_{\sigma'\vec{k}'}\delta\left(\vec{k}'-\vec{k}+\vec{q}\right)x_{\vec{q}j} + \hat{H}_{\mathrm{h\text{-}p\text{-}e}}}_{\hat{H}_{\mathrm{p\text{-}e}}}$$

Containing two sub-systems, namely the phononic one (first two terms in the 1st line represent the harmonic contribution, the third one the first two anharmonic and the last term includes higher phononic terms) and the electronic one (first two terms in the 2nd line). These interact with each other via $\hat{H}_{\mathrm{p-e}}$, describing the electron-phonon coupling (2nd line, last two terms with linear and higher coupling). With such a Hamiltonian and concepts derived by Landau-Lifshitz one can determine the order of the phase transition and the physical key parameters and learn, how to modify the transition.

We are thankful for support through the EU's Horizon 2020 research and innovation program (grant No. 899598, PHEMTRONICS).

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Mapping local thermoelectric properties of MXenes via scanning thermal microscopy

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Developing high-performance thermoelectric materials and devices that can directly convert heat into electricity has attracted increasing research. Two-dimensional (2D) materials have great potential for next-generation thermoelectric devices due to their unique physical properties and tunable structure. MXenes are a new family of 2D materials consisting of transition metal carbides and nitrides, which are predicted to show outstanding thermoelectric properties based on theoretical calculations, but few experimental studies have been performed so far. Realizing the improvement in the properties and devices performance requires understanding and controlling the MXenes local properties and structure. Scanning thermal microscopy (SThM) is a powerful tool that provides effective local thermoelectric measurements with micro/nano-scale spatial resolution. Here we study the thermoelectric properties of MXenes (e.g., Ti_3C_2, Mo_2CF_2, $TiCO_2$) by using SThM to map the local thermovoltage and temperature distribution. In detail, we first develop multiple MXenes devices with different thickness, geometry, and local defects, and then map their local Seebeck and Peltier effects, revealing the structurally dependent change in the Seebeck coefficient. The local thermoelectric properties of MXenes are important for in-depth understanding and optimizing its thermoelectric performance. The results of this study will open a path to develop novel high-performance thermoelectric materials and devices.

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Toward Understanding Thermal and Electric Properties of Single Molecular Junctions and Self-Assembled Monolayers

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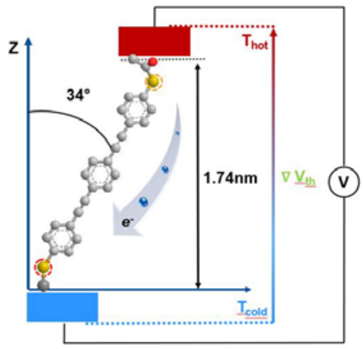
Over the last years, implanting organic molecules in devices is continuously attracting large attention because of their small size (nm scale), tunable electronic and thermal properties by manipulating individual atoms. Therefore, it is obvious to extend the field of thermoelectrics using molecules to cool devices and sensors very locally. A single layer of well-organized molecules is formed and realized by the self-assembly mechanism, which allows molecular moieties to be adsorbed spontaneously on a surface producing large domains.

This motivated us to report here about the characterization of self-assembled oligo phenylene ethynylene dithiol molecules (OPE3), and some specifically modified forms by mainly adding side groups to it on gold surfaces by means of X-ray photoelectron spectroscopy (XPS), reflected electron energy loss (REELS), and ultraviolet photoelectron spectroscopy (UPS). The results show that the unsubstituted OPE3 has a high densely packed SAM with a thickness 1.7 nm, while the presence of substituents, attached to the middle ring, led to variation of the SAM film thickness. This indicates changes in the geometric configuration of the π stacking of OPE3 especially, tilt angle and packing densities. Parent OPE3 REELS spectrum shows a band gap value of 2.01 eV which is totally different than the reported value in the literature [1].



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Novel probe for heat transport measurements in atomic and single molecule junctions

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In the realm of experimental physics, single atom[1] and molecule[2] are often regarded as ideal platforms for both fundamental research and device minimization. These nanoscale systems often exhibit peculiar quantum properties, attracting increasing attention from scientists. Electric charge transport has been systematically studied at the nanoscale level and interesting physical phenomena have been discovered[3,4]. Yet as importantly, heat transport remains largely unexplored in the single atom and molecule limit. Studying quantum properties of heat transport would possibly break our previous understanding of classical physics. However, exploring thermal conduction properties at the nanoscale presents difficult experimental challenges in terms of thermal sensitivity and mechanical stability[5,6]. Thus, only few experimental studies on the thermal transport of atomic contacts and single-molecule junctions are available currently. To circumvent these challenges, we fabricated a novel scanning probe sensor with integrated nanoscale thermocouples based on pulled quartz pipettes. Our design combines the vacuum-based scanning tunneling microscopy break-junction technique with electrical and thermal sensors placed directly at the probe-sample contact. This method opens new paths to measure heat transport mechanism in nanoscale structures.

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Thin Film Diamond Nano-photonics and its quantum Application

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Exploiting quantum effects of light matter entanglement has been limited to a small number of qubits and has only been performed in tabletop experimental setups consisting of a large number of macroscopic components Diamond is a potential candidate for the realization of quantum information technology because it encompasses optically active color centers with long-lived spin coherence and material properties that permits for the efficient use of photons and phonons as quantum information carriers. It has a large bandgap, allowing for optical transitions in defect centers. Also, diamond naturally has low number of nuclear background spins (98.9% in natural diamond is spin 0), realizing a magnetic vacuum.

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NFRHT Enhancement via External Magnetic Fields

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Radiative heat transfer between a flat SiC surface and an InSb nanosphere can be increased when we apply an external magnetic field. This happens as we couple the plasmonic resonance of the nanosphere with the polaritonic resonance of the surface, achieving an enhancement of two orders of magnitude compared with the same setting in the absence of an external magnetic field.[1]

Magnetoplasmons have been widely studied in nanoparticles; for instance, nanospheres display an analogous behavior to atoms in an external magnetic field. We observe a splitting of the resonance into two new modes, where the resonance frequency of these modes shifts as we modify the external magnetic field (Plasmonic Zeeman Effect). [2] This allows us to tune the new plasmonic modes of the nanosphere. By choosing an adequate magnetic field, we can couple one of these with the phonon-polariton frequency of the surface, thus obtaining the enhancement.

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GW + NEGF method for transport through nanostructures

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In conventional DFT+NEGF calculations, the electronic structure of density functional theory (DFT) is combined with the non-equilibrium Green's function (NEGF) approach to calculate the electronic transport through atomic and molecular contacts. Unfortunately, electronic excitation energies determined by DFT are not very accurate, especially if unoccupied states are concerned, which can lead to larger deviations from experimental observations [1]. Inspired by previous work [2] and based on recent implementations of the GW approximation in TURBOMOLE [3], we have a method to compute charge transport properties of nanostructures more accurately, as we will present.

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Correlation between thermal, optical and electrical conductivities in Azo-dyes Functionalized Polymers

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We present investigation of optical, electrical and thermal energy transfer inside the thin films of novel methacrylic polymers with 8-hydroxyquinoline azo-dyes in side-chain using two different pump-probe based photothermal measurement methods, thermal lens (TLs) and beam deflection (BDs) spectroscopy. The cross-plane thermal diffusivity and thermal conductivity were measured by BDs and TLs techniques. The highest thermal diffusivity obtained for the capazo8 (NO2) substituent while, the lowest magnitude has belonged to the capazo1 (OCH3) which is donor nanopolymer [Table1]. Additionally, Optical transition type (direct) of thin films was determined and direct optical band gaps were obtained. The lowest optical bandgap was obtained for capazo9 N(CH3)2. On the other hand, the highest direct optical band gap was obtained for capazo6 (CF3). Similarly, electrical and optical conductivity curves were investigated [figure1]. Finally, the conductivity properties of the films of samples were also investigated.

Table 1. measured thermal diffusivity and thermal conductivity using BDS method

Sample	D, mm2s-1	K,W/mk	$\alpha \times 10^5$
Capazo1	6,36E-01	0,978	56
Capazo6	6,88E-01	1,06	40
Capazo12	7,32E-01	1,128	77
Capazo10	8,18E-01	1,26	58
Capazo9	8,56E-01	1,32175	23
Capazo8	1,16E+01	1,7934	67

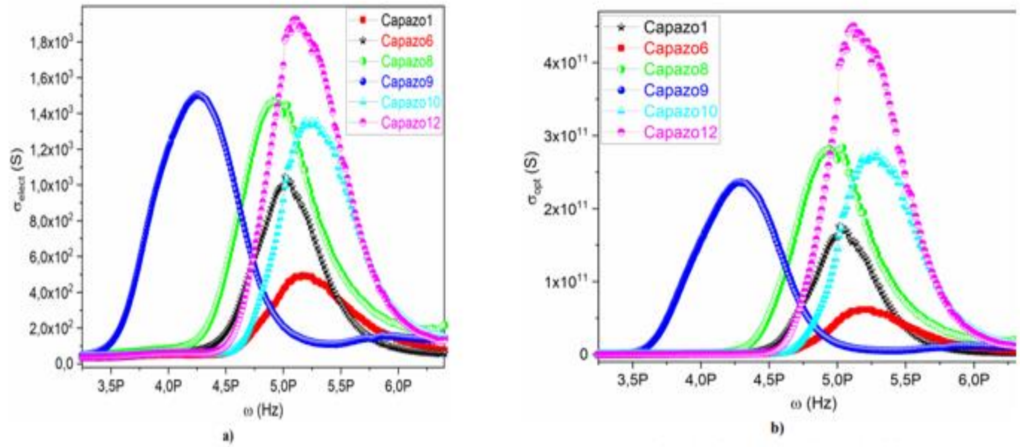

Figure 1 The **a**) electrical and **b**) optical conductivity curves

Coupling function versus phononic density of states

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Open quantum systems theory models the interaction of a quantum system with an environment. It provides the tools to calculate heat exchange of the system to the environment, consisting of phonons and electrons for example, as well as entropic terms.

In this work, we present a method of inferring the coupling between a generic system and its bosonic (e.g., phononic) environment from the experimentally measurable density of states (DOS). We use this approach and match an experimentally measured phonon DOS to a series of Lorentzian coupling functions, allowing us to determine coupling parameters for gold, yttrium iron garnet, and iron. The results illustrate how to obtain material-specific dynamical properties, such as memory kernels, and provide more accurate modelling of relaxation dynamics. Applications include, for example, quantum information processing with spin systems on the nanoscale that are damped by coupling to the crystal lattice [2] and local temperature probing with nitrogen-vacancy centers whose coherence lifetime in optical transitions is also limited by interaction with phonons [3].

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Extinction of covered ellipsoidal nanoparticles

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Plasmonic nanostructures provide an interesting platform for localized heating, field enhancement and light-matter-interaction. If a nanoparticle is covert with a thin absorbing layer, theory predicts a resonance that is not seen in experimental extinction spectra [1, 2]. To understand this issue, we analyse the distribution of electric fields and energy dissipation in and around an ellipsoidal nanoparticle. Calculations are done for gold Nano particles covered with a few nm thick absorbing layer. At the spurious resonance the field is highly localized in this layer, suggesting that strong coupling to the molecular exciton is possible at the few-photon level. We compute the impact of an effective medium approach on the calculated spectra and show, that the effective medium approach can suppress the spurious resonance.

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Measurement of Thermal Boundary Conductance (TBC) by means of Modulated-Photo Thermal Radiometry technic (M-PTR)

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In the past few decades, we saw the development of micro and nano electronic. In those devices the thermal transport can be highly impacted by nanoscale and interfacial phenomena. With the reduction of the size of these devices, the Thermal Boundary Resistance (TBC)[1], or its inverse, the Thermal Boundary/Kapitza Resistance becomes predominant. It represents the drop of temperature at an interface between two materials, when inducing a thermal gradient in both the materials.

The goal of this work is to measure the thermal boundary conductance directly, by means of a Modulated-Photo Thermal Radiometry set-up (M-PTR)[2]. The concept of such an experimental measurement, is to alternatively heat a sample with a modulated laser and to collect the complex temperature surface signal via its IR emission. Finally the signal is analyzed thanks to a Fourier model and inverse problem (Gauss-Newton) to extract different thermal parameters. One of those is the TBC.

A research project is conducted to study the influence of the electrical properties on the TBC. To do so, COMSOL simulations were made to optimize the geometry, and thus the electrical transport across the sample where the M-PTR measurement is made. A conclusion was found on the sample geometry, and those sample are composed of differently doped silicon substrate (p-doped, n-doped, and intrinsic) coated with a 30 nm thick titanium layer as a transducer, for laser beam absorption and IR emission. Then, they will be analyzed with and without operando bias to see if polarization and electron transport across the junction influence the interfacial thermal transport. A temperature study is also planned in the future.

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Sphere Probes for Scanning Thermal Microscopy

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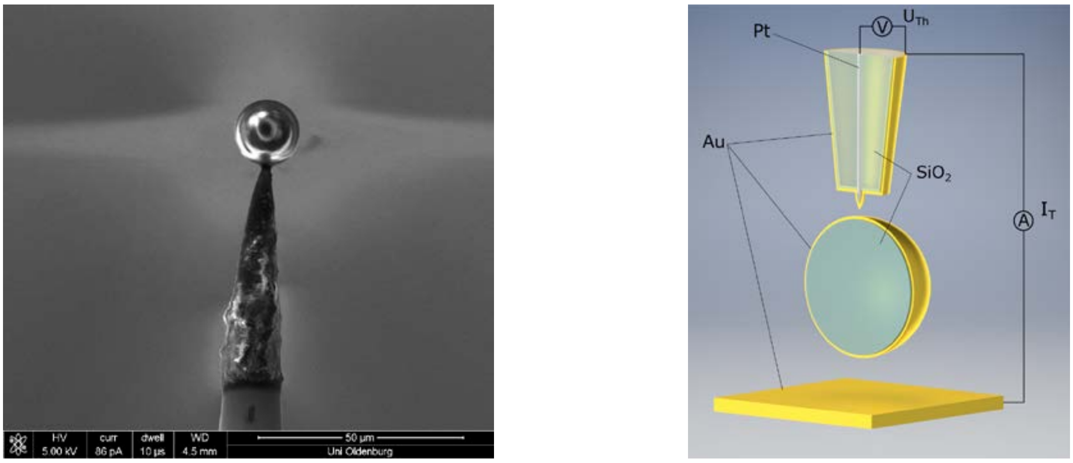
Scanning thermal microscopes based on STM (Scanning Tunneling Microscopes) and AFM (Atomic Force Microscopes) have been used for years to observe near-field mediated heat transfer. Using custom-built coaxial thermocouple tips in an STM setup, spatially highly resolved heat transfer measurements, such as the giant heat transfer at distances of a few nanometers, are possible [1]. The total heat transfer between a spherically approximated tip and a sample is expected to depend on the square of the tip's radius [2]. By attaching a 20 µm borosilicate sphere to such a coaxial thermocouple sensor, as shown in Fig. 1, heat flux sensitivity is therefore further increased in distance-dependence measurements of the heat transfer between a cooled sample and a tip at room temperature for different materials. These sensors can be used for highly resolved radiative heat transfer measurements as well as for heat conduction measurements through self-assembled monolayers of organic molecules.



(a) (b)

Figure 1: (a) Sphere probe during glue testing. (b) Schematic of a sphere probe without glue, not to scale.

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Universal Casimir interaction and its relevance for colloidal and biophysical systems

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It has been shown in a recent experiment [1] involving two dielectric spheres in salted water, that the Casimir force between the spheres is not screened for the part induced by low-frequency transverse magnetic fluctuations. The Casimir force thus contributes to a long-range interaction at distances of about one hundred nanometers. This makes the Casimir interaction also relevant for biophysical interfaces and colloidal systems involving electrolytic solutions like saltwater.

We found that due to the finite dc-conductivity of the environment, the Casimir interaction becomes universal for large enough distances [2], meaning that it only depends on the geometrical parameters. A configuration which is dual to the one mentioned above consists of two metallic spheres within vacuum where the Casimir interaction also becomes universal in the high-temperature limit. Based on the scattering approach, we obtained exact results for the zero-frequency contribution of the Casimir interaction for the metallic spheres [3]. The calculation involves a round-trip expansion between the two spheres. Within the round-trip expansion, we also obtained approximate results for the dielectric spheres that are accurate enough for most practical applications, with no need to go through numerical computations with which we validated our results [4].

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Characterization of Nanomaterials by Means of Spatially and Frequency Resolved Photothermal Radiometry

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In this work, we desire to understand the thermal properties of anisotropic bulk and thin films as well as phase change materials (PCM) that are used in the design and fabrication of systems which depend on temperature and heat flux, such as in digital electronic devices. Common methods to measure these properties include non-contact, non-destructive optical techniques. Photothermal radiometry (PTR) is one such technique that uses a modulated laser in the visible spectrum to heat a sheet of a material that can vary in thickness from micrometers to nanometers. The sample produces an infrared response due to the excitation from the laser which is then collected by a detector and analyzed to determine the unknown thermal properties. Normally, PTR is used to measure properties solely in the direction orthogonal to the sheet's surface. However, recently it has been successfully used to measure multi-dimensional characteristics [1]. The work presented in this abstract focuses on progressing this new PTR-based method to measure anisotropic thermal properties, including thermal conductivity measurement in two dimensions (in plane and cross plane). The new system differs from a standard PTR experiment mainly in that the detector translates within a plane to probe different points across the sample so that properties can be measured multidimensionally. Then, an analytical solution for the heat equation using a Hankel transform can be fitted with the experimentally measured data using the Gauss-Newton method to solve for the unknown quantities. It is expected that these results will agree with standard PTR measurements performed on individual cross sections of the samples representing each material direction. Current challenges include programming the Hankel transform heat equation solution to match the previously established Fourier transform solution as well as system calibration. The objective of this technique and method is to be able to measure anisotropic properties of materials of interest accurately to enable the use of the next generation of materials in temperature and heat flux sensitive applications. A better understanding of the thermal properties of these materials is crucial in order to be able to properly model thermal systems and optimize designs.

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Electro- & Opto-thermal Measurements of Low Dimensional Materials

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The understanding of phonon transport phenomena in low-dimensional materials is highly significant for fundamental research and growing demands for innovative materials structures that can work in harsh environments [1]. One important example is integrated devices, where heat management has become critical for maintaining the performance and reliability of the devices [2,3]. In addition, the manipulation of phonons in solids can be exploited for various applications such as thermal diodes and thermal transistors [4]. In this regard, our research is focused on engineering and measuring phonons and phonon transport in nanostructures.

Importantly, we investigate the phononic properties of nanomaterials using different approaches including opto- & electro-thermal measurements such as Raman thermometry, ultrafast techniques, and novel suspended device methods. The present research aims to contribute to this growing area of research by exploring the thermal properties of telescopic, twin superlattice nanowires, and 2D materials. In this work, we will present the thermal rectification effect obtained on telescopic nanowires made of GaAs, we will show the characterization carried out on suspended two terminal bridges in combination with Raman thermometry. We will also show the thermal conductivity of GaAs-GaP superlattices as a function of the superlattices period, this measurement yield the crossing point between particle behavior and wave behavior of phonons at the minima in the thermal conductivity.

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Spatially resolved thermometry on metal oxide RRAM devices by means of Scanning thermal microscopy

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Self-heating and localized temperatures can be a major drawback in the principle of operation and reliability of nano- and micro-scale devices. For example, energy dissipation in memory devices is connected to some disadvantages, like reliability and energy efficiency. Understanding the underlying mechanisms is therefore essential for the evaluation, design and optimization of our electronic devices. [1]

Scanning thermal microscopy (SThM) is a scanning probe microscopy technique that allows the spatially localized characterization of heat transport characteristics with a nanoscale resolution (~50 nm). Therefore, SThM is a promising tool, which has been employed for determining local hot spots and self-heating of different types of electronic devices. [2,3]

In this work, we use SThM for the characterization of heat dissipation in nanoelectronics. Our SThM uses a thermo-resistive probe whose electrical resistance varies with temperature. This probe is utilized as a nanoscale sensor to map thermal features in our devices locally. First, we present challenges associated with the calibration of this probe in order to convert the thermally induced electrical signal in a quantitative temperature change. Afterwards we used the SThM to map the heating in TiO_x based Resistive Random Access Memory (RRAM) devices. In these devices switching is induced by the formation and disruption of highly localized conductive filaments as illustrated in Figure 1. By means of the SThM we are able to map, localize and quantify the heat originated from the filament. These maps provide insights into device operation, showing how the energy dissipates and offering new routes for developing more efficient switching mechanisms.

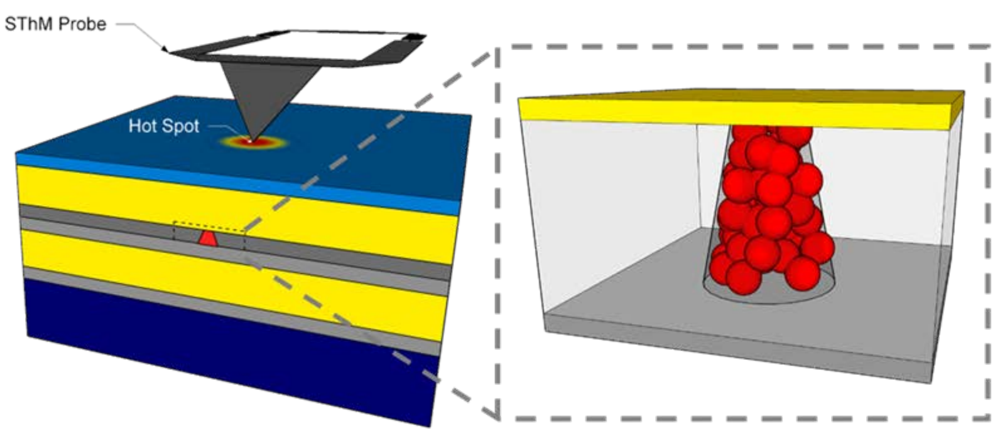

Figure 1: Illustration of the investigated material structure and measurement technique

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