International Conference on

Molecular-Scale Charge and Thermal Transport

MSCTT 2020

January 27 - 31, 2020, Engelberg, Switzerland

Book of Abstracts

Charge and thermal transport across nanostructured systems plays a role in countless disciplines, including electronics, green energy, catalysis and biochemical sensors. A symbiosis of theory, synthesis, measurement and device design is required to understand and create novel functional materials with desirable properties for future applications. Recent developments in fabrication, analytical and computational methods make it possible to study how charge carriers interact with molecules and nanostructured materials in greater detail than ever before, enabling studies of quantum effects, spin-dependent transport, light-matter interactions and thermoelectric effects at the smallest length scales. It is thus timely and desirable to strengthen inter-disciplinary interactions between theoreticians, material scientists, chemists and experimental physicists in order to overcome obstacles, clear up novel pathways and push the field forward.

The International Conference on Molecular-scale Charge and Thermal Transport will bring together world leaders in materials and chemical synthesis, in experiments on functional devices and in transport theory. Together with younger scientists, these experts will discuss recent progress, challenges and applications of newly emerging transport phenomena, and stimulate the creation of interdisciplinary collaborations within the molecular devices community.

This workshop is an initiative of the EU Consortium QuIET - Quantum Interference Enhanced Thermoelectricity.

On behalf of the organizers,

Michel Calame

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University of Oxford, UK

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University of California Los Angeles, US

Prof. Diana Dulić
University of Chile, CL

Prof. Jaime Ferrer
University of Oviedo, ES

Prof. Milena Grifoni
University of Regensburg, DE

Dr. Edmund Leary
IMDEA Nanoscience, ES

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Abstracts

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Monday, January 27. 20:30 – 21:30

Molecular electronics and plasmonics: Electrons, light and heat transport at the nanoscale

Abraham Nitzan*

*University of Pennsylvania, US

In molecular conductance spectroscopy, the current through a molecule (or molecules) connecting two metal or semiconductors electrodes is measured as a function of the applied voltage. With eye on potential technological applications, the main problems facing researchers in this field fall within the subjects of fabrication, characterization, stability, functionality and control. As a theoretical problem, one needs to deal with a non-equilibrium system open to electron and energy reservoirs, possibly under illumination. This talk will review recent progress in understanding transport in molecular junctions and the interplay between electronic transport, nuclear motion, optical and mechanical response and interaction with the thermal environment, with particular emphasis on the theoretical modeling of these phenomena.

Tuesday, January 28. 09:00 – 09:50

Switches, rotors and photon sources with single molecules on surfaces

Wulf Wulfhekel*

*Karlsruhe Institute of Technology, DE

Achieving functionality of single molecules on surfaces often requires a careful design of the molecules especially regarding the strong surface molecule interaction. We present our recent activities in using rigid platforms that selectively bind to a Au(111) substrate on top of which the functional group of the molecule is placed. In combination with low-temperature scanning tunneling microscopy (STM), we demonstrate electrostatically driven switches and chiral molecular rotors. Using a specially designed STM for light collection from the tunneling junction, we achieve extremely bright electroluminescence from charged and electrically isolated species.

Tuesday, January 28. 09:50 – 10:10

Quantum and Phonon Interference Enhanced Molecular-Scale Thermoelectricity

Hatef Sadeghi*

*School of Engineering, University of Warwick, UK

There is a worldwide race to find materials with high thermoelectric (TE) efficiency to convert waste heat in consumer electronics and server farms to useful energy. Despite several decades of development, the state-of-the-art TE materials are not sufficiently efficient to deliver viable technology platform for energy harvesting from consumers electronics or on-chip cooling of CMOS-based devices. The efficiency of a TE material is defined by a dimensionless figure of merit $ZT = S^2GT/K$, where S is the Seebeck coefficient, G is the electrical conductance, T is temperature and $K = K_{el} + K_{ph}$ is the thermal conductance due to electrons and phonons, respectively. Therefore low-K, high-G and high-S materials are needed. This is constrained by the interdependency of G, S and K. Consequently, the world record ZT is about unity at room temperature in inorganic materials which are toxic and their global supply is limited. To develop high-performance TE devices, simultaneous engineering of electron and phonon transport through nanostructured TE materials is needed. In molecular scale junctions, electrons behave phase coherently and can mediate long-range phase-coherent tunneling even at room temperature. This creates the possibility of engineering quantum interference in these junctions for thermoelectricity. In this talk, I will discuss strategies to improve the efficiency of TE materials. This includes utilising quantum interference to enhance electrical conductance and Seebeck coefficient and phonon interference to suppress thermal conductance in molecular scale junctions.

Tuesday, January 28. 10:10 – 10:30

Joule Heating and Thermovoltage in Graphene nano-constrictions

Charalambos Evangeli*, Jean Spiece, Achim Harzheim, Pascal Gehring, Sumit Tewari, James Thomas, Oleg Kolosov, Jan Mol

*Department of Materials, University Of Oxford, UK

Graphene is of great interest for both fundamental research and future technological applications, including thermal management and thermoelectric applications. We investigate joule heating in graphene nano-constrictions close to the rupture limit using a feedback control breaking mechanism. We apply Scanning Thermal Microscopy, to measure the temperature during the controlled graphene breakdown. We study the phonon assisted transport through the graphene and found that that electron-phonon scattering increases strongly with disorder. Furthermore, we map the thermovoltage of the devices at different stages of breakdown and we show that reducing the width of a graphene channel changes the Seebeck coefficient.

Tuesday, January 28. 11:00 – 11:50

Tailoring Charge Transport in Vertical Molecular Tunnel Junctions

Xiangfeng Duan*

*University of California Los Angeles, US

Molecular tunneling devices represent an attractive alternative for future electronic devices with rich functionalities beyond current scaling limits of silicon-based electronics, as diodes, switches and transistors. However, to realize these applications of molecular devices, there is an urgent need to explore new design of molecular tunnel junctions and control charge transport through these tunnel junctions. Here we report the novel design of vertical molecular tunneling junctions based on a single-layer graphene (SLG)/self-assembled-monolayer (SAM)/gold cross-plane vertical heterostructure. Since the SLG exhibits selective permeability, the charge transport in the vertical molecular tunnel junctions can be controlled through the top SLG electrode. Specifically, when molecules with destructive quantum interference (QI) effects are used to form SAMs and ionic liquid is used for generating the strong gating electric field, efficient molecular tunnel transistors can be realized by utilizing electric field transparency of the SLG electrode. The chemical or electrochemical redox reactions crossing the SLG can be used for switching the vertical tunnel junction composed of SAMs with redox-active groups. Furthermore, by utilizing the permeability of graphene to protons, the SAMs with acid groups can be converted into negatively states, which can be used for fabricating efficient molecular diodes and transistors.

Tuesday, January 28. 11:50 – 12:10

Electron transport through graphene-based molecules containing different structural defects

Lucía Palomino-Ruiz,* S. Rodríguez González, Irene R. Márquez, Vicente G. Jimenez, Silvia Castro-Fernandez, Edmund Leary, Nicolás Agraït, Alba Millán, Cristina Diaz, Juan M. Cuerva, L. A. Zotti, Fernando Martin, Araceli G. Campaña, M. Teresa González.

*University of Granada, ES and IMDEA Nanoscience Institute, ES

Structural defects can promote significant alterations in the physical properties of graphene. Understanding the relationship between different types of defects and the changes in the properties would make possible to find new and unexpected applications for defective and distorted graphene. The versatility of organic chemistry allows the synthesis of graphene-based molecules in a wide range of shapes and sizes and provides the possibility of including different defects in selected positions. In this work we have studied the influence of two kind of structural defects in the electron transport properties. Specifically designed for that purpose, we have synthesized a family of polyaromatic structures containing 7-membered rings and another incorporating B and N atoms, both with thiomethyl (-SMe) groups, which play the role of anchors to the electrodes in the course of the electron transport experiments. We have used the scanning tunneling microscopy break-junction (STM-BJ) technique for studying their electronic conductance and that of their defective-free analogues at the single molecule scale. The obtained experimental values have been compared and theoretical calculations has been also carried out in order to give a deeper understanding of the impact of these defects on the electronic properties.

Tuesday, January 28. 12:10 – 12:30

Understanding resonant charge transport through weakly coupled single-molecule junctions

James Thomas,* Bart Limburg, Jakub K. Sowa, Kyle Willick, Jonathan Baugh, Erik M. Gauger, G. Andrew D. Briggs, Harry L. Anderson, Jan A. Mol.

*University of Oxford, UK

Off-resonant charge transport through molecular junctions has been studied since the advent of single-molecule electronics and is well understood within the framework of the non-interacting Landauer approach. Conversely, a qualitative and quantitative understanding of the resonant transport regime has proven more elusive. We find that zinc-porphyrins interfaced with graphene electrodes through pi-pi stacking interactions exhibit charge transport in the weak-coupling regime. Therefore, by studying the tunnelling current as a function of bias and gate voltage in a three-terminal device, we can study resonant, sequential charge transport through the molecular junction in great detail. We experimentally demonstrate an inadequacy of Landauer theory and the conventional single-mode Franck–Condon model. We model overall charge transport as a sequence of non-adiabatic electron transfers, and show that the transport properties of our molecular junctions are determined by a combination of electron–electron and electron-vibrational coupling, and are sensitive to interactions with the local environment. Furthermore, we use temperature-dependent transport data to assess the importance of nuclear tunnelling and examine the suitability of semi-classical Marcus theory as a description of charge transport in molecular devices. Electronic and magnetic properties of single-molecule transistors depend critically on the molecular charge state. This is often difficult to assign in each Coulomb-blocked region due to variability in the work-function of the electrodes. A result of electron-electron interactions and asymmetric molecule-electrode coupling means that the molecular charge state can be assigned by simply observing tunnel-current asymmetries in sequential tunnelling regions. This provides a simple and fast method to assign the charge state of the molecular species in the Coulomb-blocked regions that is applicable at room temperature. We demonstrate that charge-state assignments determined in this way are consistent with those obtained from measurements of Zeeman splittings. Correct assignment of charge states and greater understanding of resonant transport allows researchers to better understand the fundamental charge-transport properties of single-molecule transistors.

Tuesday, January 28. 14:00 – 14:50

Electric and thermoelectric properties of conjugated oligomers at the single molecule level

Edmund Leary,* B. Limburg, A. Alanazy, S. Sangtarash, I. Grace, K. Swada, L. J. Esdaile, M. Noori, M. T. Gonzalez, G. Rubio-Bollinger, H. Sadeghi, A. Hodgson, N. Agrait, S. J. Higgins, C. J. Lambert, H. L. Anderson, R. J. Nichols.

*IMDEA Nanociencia, ES

The combined measurement of electrical and thermoelectric properties of conjugated oligomers provides an extremely detailed view of charge flow across single molecule junctions in break junction experiments. We have used scanning tunneling microscopy-based methods to explore the current-voltage and thermoelectric response of various families of molecules, uncovering rich behavior in each system. The systems I will discuss are as follows: Porphyrin wires. We have studied two families, one with flexible butadiyne spacers between the porphyrins, the other in which the porphyrins are fused in a coplanar arrangement.[1] Fusion results in a dramatic reduction of the HOMO-LUMO gap compared to the butadiyne-family. The consequence of this is remarkable high-bias behavior where the conductance increases with length yielding a negative beta value. The butadiyne-family display larger Seebeck coefficients and both families display an odd-even effect. Reasons for this behavior will be discussed. Oligoyne wires. We have studied a range of oligoynes containing up to eight consecutive triple bonds. Due to their simplicity, they represent an ideal system to test models of charge transport at the single molecule level. Using their I-V response and Seebeck coefficients, one can compare these with simple transport models which seem to describe these properties well. Our results support the Landauer picture of charge transport. Cumulene wires. In contrast to oligoynes, cumulenes, having close to zero bond-length alternation, can be viewed as “metallic” for an infinitely long chain. We have studied the conductance of a series of cumulenes where the number of consecutive C=C bonds in the core is n=1, 2, 3, and 5. The family has a rather unusual length dependence, where the n=1, 3 and 5 have virtually identical conductance.[2] The voltage dependence shows that cumulene junctions can support high currents in the microampere range, where the maximum current is most likely limited by the contact.

[1] J. Am. Chem. Soc. 2018 140 (40), 12877-12883.
[2] Angew. Chem. 2019, 131, 8466.

Tuesday, January 28. 14:50 – 15:10

Electron and thermal transport at the nanoscale in molecular films. Two case studies: polyoxometalates and benzothiophene derivatives

Dominique Vuillaume,* D. Guerin, M. Gueye, S. Lenfant, Laurans, K. Dalla Francesca, F. Volatron, A. Proust

*IEMN, CNRS, Univ. Lille, FR

Polyoxometalates (POMs) are nano-scaled molecular oxides endowed with a remarkable structural diversity and outstanding magnetic and/or redox properties. This makes them fascinating magnetic and/or electro-active molecules to be integrated in functional materials such as multi-level non-volatile memories or other nano-electronic and spintronics devices.[1,2] Yet the shaping of POMs layers onto electrodes is still a sticking point, albeit essential to improve the control of the POMs/electrode interface and hence the ultimate electrical properties. We have developed several routes to the deposition of POMs: by electrostatic deposition of POMs onto a preformed and charged SAM on Au or by direct covalent grafting of POMs onto n-Si(100)[3]. We will present and discuss the transport properties of these molecular junctions,[4,5] assessed at several scale lengths (Hg drop, conducting-AFM on monolayers and nanodot-molecule-junctions).[6,7] We used the scanning thermal microscope (SThM) to study the thermal conductance of films of alkylated benzothieno-benzothiophene (C8-BTBT-C8) with a marked "staircase" topography up to 400 nm. In contrast, the local thermal resistance, Rth, shows a weak thickness dependence. This feature will be discussed considering distance-dependent thermal conductivity and/or interfacial vs. bulk thermal conductivity.

[1] Chen, X. L.; Zhou, Y.; Roy, V. A. L.; Han, S. T. Adv. Mater. 2018, 30 (3), 1703950. [2] Tanaka, H.; Akai-Kasaya, M.; TermehYousefi, A.; Hong, L.; Fu, L. X.; Tamukoh, H.; Tanaka, D.; Asai, T.; Ogawa, T., Nature Communications 2018, 9, 2693. [3] Volatron, F.; Noel, J. M.; Rinfray, C.; Decorse, P.; Combellas, C.; Kanoufi, F.; Proust, A. J. Mater. Chem. C 2015, 3 (24), 6266-6275. [4] Laurans, M.; Francesca, K. D.; Volatron, F.; Izzet, G.; Guerin, D.; Vuillaume, D.; Lenfant, S.; Proust, A., Nanoscale 2018, 10, 17156-17165. [5] Dalla Francesca, K. ; Lenfant, S. ; Laurans, M. ; Volatron, F. ; Izzet, G., Humblot, V., Methivier, C., Guerin, D., Proust, A., Vuillaume, D. Nanoscale 2019, 11, 1863-1878. [6] Smaali, K.; Clément, N.; Patriarche, G.; Vuillaume, D. ACS Nano 2012, 6, 4639–4647. [7] Clément, N.; Patriarche, G.; Smaali, K.; Vaurette, F.; Nishiguchi, K.; Troadec, D.; Fujiwara, A.; Vuillaume, D. Small 2011, 7, 2607–2613.

Tuesday, January 28. 15:10 – 15:30

Electrically transmissive SAM on gold

Lucia Herrer,* A. González-Orive, S. Marqués-González, S. Martín, R. J. Nichols, J. L. Serrano, P. J. Low, P. Cea

*University of Zaragoza, ES

The search for robust and reliable metal-molecule contacts based on self-assembled monolayers (SAMs) represents an on-going issue in the development of active molecular materials or components on metal substrates. Surface-molecule interactions upholding surface-functionalised clusters, metal nanoparticles (NPs) and electrodes, have great promise in different areas including microelectronics, microelectromechanical systems, molecular electronics, surface protection, sensing, electrochemistry, and electrocatalysis among others.1-3 In this contribution, a self-assembled monolayer film of an OPE (oligo phenylene ethynylene) derivative is described, having a direct activation through an ethynyl moiety to a gold, Au (111), electrode. The molecular structure allows to fabricate well-ordered and densely packed monolayers showing a free-alkyne top surface available for further post-assembly functionalization of the film. In contrast with gold-supported monolayer films of comparable OPE derivatives but incorporating other anchoring groups, the electrochemical measurements performed using different redox probes, reveal that this molecular junction presents a remarkably low charge transfer barrier. Additionally, a very low voltage transition (Vtrans = 0.51 V) from direct tunneling (rectangular barrier) to field emission (triangular barrier) is indicative of a low tunneling barrier and is consistent with the facile charge transport observed through the C-Au contacted SAM. These properties have been demonstrated via a complete set of experimental data, including QCM, AFM, STM and CV.4 The observed phenomenon could offer new avenues for the fabrication of highly conductive large-area monomolecular films and may find future applications in the fabrication of electrochemical sensors and immunosensors, plasmonics, electrocatalysis, electroanalysis, and photovoltaics.

[1] A. Vilan, D. Aswal, D. Cahen, Chem. Rev., 2017, 117, 4248.
[2] P. Maity, S. Takano, S. Yamazoe, T. Wakabayashi, T. Tsukuda, J. Am. Chem. Soc., 2013, 135, 9450.
[3] P. T. Mathew, F. Fang. Engineering, 4, 2018, 760.
[4] L. Herrer, A. González-Orive, S. Marqués-González, S. Martín, R. J. Nichols, J. L. Serrano, P. J. Low, P. Cea. Nanoscale, 2019, 11, 7976."

Tuesday, January 28. 16:00 – 16:50

QuIET: Quantum Interference Enhanced Thermoelectricity

Nicolás Agraít*

*Universidad Autónoma de Madrid, ES

In this talk I will give an overview of our EU project QuIET. The goal of QuIET is to demonstrate that quantum interference in molecular junctions can lead to enhance thermoelectric properties and can be exploited in massively-parallel arrays of molecules to design ultra-thin thermoelectric devices.
QuIET is a highly interdisciplinary project involving synthesis, transport measurements and theoretical modelling. The QuIET consortium is formed by the Universidad Autónoma de Madrid (Spain), Lancaster University (UK), Delft University of Technology (The Netherlands), the University of Durham (UK), IBM-Zurich (Switzerland), Basel University (Switzerland) and SWISS FEDERAL LABORATORIES FOR MATERIALS SCIENCE AND TECHNOLOGY (EMPA) (Switzerland).

Tuesday, January 28. 16:50 – 17:10

Clustering methods for data analysis in molecular junctions

Maria El Abbassi,* Mickael perrin Patrick Zwick Alfredo Rates Davide Stefani Alessandro Prescimone Diana Dulic Marcel Mayor Michel Calame Herre van der Zant

*TU Delft, NL

Single-molecule measurements are intrinsically stochastic in nature, requiring the acquisition of large datasets to gain insight into the generic electronic properties of the molecule under study. For example, in the case of break-junction measurements, the most probable conductance value of the molecule is often extracted from the conductance histogram built from thousands of 'breaking' traces. In this talk, I will briefly introduce unsupervised clustering methods that will be employed to improve the analysis of molecular measurements. Three different examples will be shown: 1- Improvement of the determination of the conductance of oligo(phenylene ethynylene)dithiol molecules measured in a mechanically controlled break-junction (MCBJ) measurements [1], 2- Identification of the different electronic paths through a porphyrin molecule [2], 3-Quantitative estimation of sample-to-sample fluctuations [3].

[1] D. Cabosart et al., Appl. Phys. Lett. 114, 143102 (2019)
[2] M. El Abbassi et al., Chem. Sci., 10, 8299-8305 (2019)
[3] M. El Abbassi et al., Nature Nanotechnology, 14, 957–961 (2019)

Tuesday, January 28. 17:10 – 17:30

Charge Transport in Semiconductors Assembled from Nanocrystals

Nuri Yazdani*

*ETH Zurich, CH

The potential of semiconductors assembled from nanocrystals (NC semiconductors) has been demonstrated for a broad array of electronic and optoelectronic devices, including transistors, light emitting diodes, solar cells, photodetectors, thermoelectrics, and phase charge memory cells. Despite the commercial success of nanocrystals as optical absorbers and emitters, applications involving charge transport through NC semiconductors have eluded exploitation due to the inability to predictively control their electronic properties. In the work presented here, we perform large-scale, ab-initio simulations to understand carrier transport, generation, and trapping in NC-based semiconductors from first principles. We use these findings to build a predictive model for charge transport in NC semiconductors, which we validate experimentally. Our new insights provide a path for systematic engineering of NC semiconductors, which in fact offer previously unexplored opportunities for tunability not achievable in other semiconductor systems.

Wednesday, January 29. 09:00 – 09:50

Harvesting heat from electrons in nanowires

Heiner Linke,* Martin Josefsson, Artis Svilans, I-Ju Chen, Steven Limpert, Adam M. Burke, Eric A. Hoffmann, Sofia Fahlvik, Jonatan Fast, Claes Thelander, Martin Leijnse

*NanoLund and Solid State Physics, Lund University, SE

It has been known for some time that a perfect (delta-function) energy filter allows, in principle, thermal-to-electric energy conversion near ideal (Carnot) efficiency. [1,2] I will introduce this concept and report on a recent experiment where we realized a near-ideal quantum-dot heat engine in devices based on single InAs/InP heterostructure nanowires, realizing power production with Curzon-Ahlborn efficiency (> 50% of Carnot efficiency) at maximum power settings, and reaching more than 70% of Carnot efficiency at maximum efficiency settings [3]. This proof-of-performance of efficient energy harvesting from electrons is directly relevant to the concept of hot-carrier or thermophotovoltaics, where the aim is to boost energy conversion efficiency by harvesting heat from non-equilibrium electrons [4]. I will present our progress towards implementing this principle in heterostructure nanowires [5].

[1] Mahan & Sofo, PNAS 93, 7436–7439 (1996).
[2] Humphrey, T. E., Newbury, R., Taylor, R. P., & Linke, H. (2002). Phys Rev. Lett. 89 116801 (2002).
[3] Martin Josefsson, Artis Svilans, et al.: Nature Nanotechn. 13, 920–924 (2018)
[4] S. Limpert, S. Bremner, and H. Linke: New J. Phys. 17, 095004 (2015)
[5] S. Limpert, et al.: Nanotechnology 28, 43 (2017)

Wednesday, January 29. 09:50 – 10:10

Raman Spectroscopic Investigation of Graphene Nanoribbon Thin Films

Jan Overbeck,* G. Borin Barin, C. Daniels, M. L. Perrin, O. Braun, P. Ruffieux, V. Meunier, R. Fasel, M. Calame

*Swiss Federal Laboratories for Materials Science and Technology (Empa), CH

Graphene nanoribbons (GNRs) exhibit an electronic bandgap due to the lateral confinement of charge carriers and edge effects. They can be fabricated by bottom-up on-surface synthesis from molecular precursors resulting in atomically precise structures [1]. This approach promises tunable optical and electronic properties [2]. Their integration into functional devices will require an in-depth understanding of their structural properties, in particular after transfer from their metallic growth substrates to the target device substrate. We use Raman spectroscopy to characterize GNRs throughout the device fabrication process. Toward that end, we employ large area Raman mapping and have developed optimized device substrates exhibiting interference enhancement [3]. In this way, we have identified new low intensity Raman modes that provide information on the geometry of GNRs. In particular, a newly identified longitudinal compressive mode (LCM) can be used to investigate the length of bottom-up synthesized GNRs, probe the effects of device processing, and the interaction of GNRs with different types of substrates [4]. We further show how these measurement approaches can be translated to the investigation of other thin films.

[1] Cai, J. et al., Nature 466, 470–473, (2010)
[2] Chen, Y.-C et al., ACS Nano 7, 7, 6123–6128, (2013)
[3] Overbeck, J. et al., phys. stat. sol. (b), doi: 10.1002/pssb.201900343, (2019)
[4] Overbeck, J. et al., ACS Nano, doi: 10.1021/acsnano.9b05817, (2019)

Wednesday, January 29. 10:10 – 10:30

Contact Metal Effects on the Conductance of -dithiol Linked Single-molecule Junctions

Keisha Michael,* Chaolong Yang, Walther Schwarzacher

*University of Bristol, UK

Its resistance to oxidation makes gold a highly convenient contact metal for use in molecular electronics, and this is reflected in the extensive published literature on gold-single-molecule-gold junctions. However, alternative contact materials such as the ferromagnetic first row transition metals create the opportunity to probe new effects including spin-dependent transport. To date, work on single-molecule junctions incorporating first row transition metals has been limited because of their tendency to oxidise in ambient conditions. Here we have used a combination of break junction methods (STM break junction and mechanically controllable break junction) to show for the first time that it is possible to form reproducible cobalt - single-molecule - cobalt junctions in air. Crucially, their conductance is consistent with that measured under electrochemical control to avoid cobalt surface oxidation. Furthermore, we show that using cobalt electrodes to form metal -pentanedithiol - metal single-molecule junctions results in a conductance that is an order of magnitude higher than that measured when using gold electrodes, though the same is not true for metal- benzenedithiol - metal junctions. The ability to measure single-molecule conductances with ferromagnetic electrodes in ambient conditions opens up new possibilities for molecular spintronics and its applications.

Wednesday, January 29. 11:00 – 11:50

A nanoengine powered by single electrons

Andrew Briggs*

*University of Oxford, UK

Electrons flowing one at a time through a carbon nanotube can spontaneously induce mechanical oscillations. This represents an extreme limit of electron-phonon coupling for a heat engine. Although the back-action from electron tunnelling is stochastic, under sufficiently strong coupling it can create self-sustaining mechanical oscillations. This can be thought of as damping associated with a Breit-Wigner resonance in a regime where it becomes negative due to asymmetries in the tunnelling barriers. The output of the oscillator is coherent. It has similarities with laser emission, including injection locking, classical squeezing through anharmonicity, and frequency narrowing through feedback. The engine provides a platform for nanoscale non-equilibrium thermodynamics, both classical and quantum.

Yutian Wen, N. Ares, F. J. Schupp, T. Pei, G. A. D. Briggs & E. A. Laird. A coherent nanomechanical oscillator driven by single-electron tunnelling. Nature Physics (2019) doi:10.1038/s41567-019-0683-5.

Wednesday, January 29. 11:50 – 12:10

Universal approach for unsupervised data classification

Mickael Perrin,* Maria El Abbassi, Michel Calame, Herre S. J. van der Zant

*Swiss Federal Laboratories for Materials Science and Technology (Empa), CH

Data clustering is a powerful method for analysis of datasets and identification of characteristic features occurring throughout the dataset without a priori knowledge of the structure of the data. Here, we introduce a universal approach for unsupervised data classification that can be applied to any dataset consisting of univariate measurements. Our method relies on a two-step procedure, the first one being the conversion of each measurement into a feature space vector, and the second one a clustering algorithm used for the partitioning of the feature space. We investigate a large range of feature space construction methods and clustering algorithms, and extensively benchmark them against simulated datasets with known classes, with some combinations yielding accuracies close to 93%. Further on, the most promising feature space construction method and clustering algorithms are applied to three types of different experimental data sets. Finally, we employ 34 internal and relative cluster validation indices in order to determine the number of classes, a critical step in the clustering algorithm. Our method is ideally suited for a wide range of measurement types in the field of nano-electronics, such as current-voltage characteristics, mechanically controllable breaking junction conductance-displacement traces, atomic force microscope measurements and spectroscopy curves (Raman, infrared, scanning tunneling spectroscopy, etc...). Moreover, this approach is not limited to experimental data, but can readily be applied to theoretical datasets, such as electron transmission curves.

Wednesday, January 29. 12:10 – 12:30

A Transfer Learning approach for unsupervised classification of molecular conductance traces

Anton Vladyka,* Tim Albrecht

*School of Chemistry, University of Birmingham, UK

Nanometer-sized objects such as individual organic molecules can exhibit a potentially large number of configurations when 'wired' between two metallic electrodes. Therefore comprehensive electrical characterization of molecules requires to repeat measurements for hundreds or even thousands of times and to perform statistical analysis of measured data. Processing of individual traces is not sufficient and can introduce human bias into the data interpretation therefore to extract differences in microscopic behavior of molecules different unsupervised approaches are used to separate data into different clusters [1, 2, 3]. Here we demonstrate how the neural network designed for image recognition – one of the most advanced modern data classification techniques – can be adapted for unsupervised classification of conductance traces, allowing different, physically meaningful sub-populations to be identified otherwise gone unnoticed [4]. For example, this approach effectively separates conductance traces formed by several molecules in parallel from the traces corresponding to predominantly single molecular junctions.

[1] M. Lemmer et al., Unsupervised vector-based classification of single-molecule charge transport data. Nat. Commun. 7, 12922 (2016).
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[4] A. Vladyka, M. Calame, T. Albrecht, manuscript in preparation.

Thursday, January 30. 09:00 – 09:50

Designing of a "perfect" porphyrin molecule for the Mechanically Controllable Break Junction Experiments

Diana Dulić*

*FCFM, Universidad de Chile, CL

The biggest challenge of molecular electronics is to condense the functionality of an electronic device into a single molecule and to exploit the functional versatility offered by the chemical diversity of molecules for electronic device purposes. Porphyrins and their related macrocycles are promising building blocks for the construction of bio-inspired molecular devices. Nature itself offers magnificent examples of porphyrin usefulness, such as activating and transporting molecular oxygen in mammals and harnessing sunlight in plant photosynthetic systems. In spite of their potential, obtaining well defined single-molecule conductance features is a difficult task. Due to p-stacking porphyrins can form a variety of junction configuration, leading to a large spread in condpuctancevalues using the mechanically controllable break junctions (MCBJ) technique. This limits further progress in investigating the molecular functionalities on a single molecule level in porphyrin molecules. In this presentation, I will show that by close interaction between synthetic chemists and physicists a "perfect" porphyrin molecular design for mechanically controllable break junctions can be achieved, leading to well defined, highly conducting molecular junctions. This opens further prospects for "porphyronics"– porphyrin-based molecular electronics.

Thursday, January 30. 09:50 – 10:10

Simultaneous conductance and thermopower characterization of single-molecule junctions

Laura Rincón-García,* Edmund Leary, M. Teresa González, Gabino Rubio-Bollinger, Nicolás Agraït

*Universidad Autónoma de Madrid, ES

The final goal of developing molecular electronic devices with improved capabilities requires first the fundamental understanding of charge transport through single-molecule junctions. Thermoelectric properties of these systems result especially interesting due to potential applications in waste heat recovery or local cooling and because they provide complementary insights about the transport mechanisms, not accessible characterizing only the electrical conductance. A lot of effort has been done during the last ten years in this direction, studying the effect on the thermoelectric response of different factors such as molecular length, anchor groups, electrode material or conjugated versus nonconjugated bridging units. Using a home-made scanning tunnelling microscope (STM) adapted to apply voltage and temperature differences across single-molecule junctions formed with the STM-break-junction technique, we have performed simultaneous characterization of conductance and thermopower of molecular junctions in ambient conditions and at room temperature. The combination of these measurements offer complementary and valuable information about their transport properties, as it is going to be shown for some of the latest molecules investigated.

Thursday, January 30. 10:10 – 10:30

A unified theory of thermal transport in crystal and glasses, and a generalization of Fourier's law to heat hydrodynamics

Michele Simoncelli,* Nicola Marzari

*École Polytechnique Fédérale de Lausanne, CH.

We develop a unified theory of thermal transport [1] that encompasses both the particle-like heat conduction mechanisms of (ordered) crystals [2] and the wave-like conduction of (disordered) glasses [3], while also covering all the intermediate regimes. We explain the opposite trend of the temperature-conductivity curve of crystals and glasses, and solve the long-standing problem of rationalizing why some complex crystals (e.g. thermoelectrics) display glass-like heat-transport properties. The accuracy of the present formulation is showcased on several materials, including crystals for thermoelectric energy conversion [4] and glasses. We also examine the emergence of hydrodynamic thermal transport in crystals, showing that the underlying physics can be coarse-grained into two novel mesoscopic "viscous heat equations" [5] that include Fourier's law and second sound (i.e. heat propagation as a coherent wave) as limiting cases. This mesoscopic formulation explains why in electronic or phononic devices heat propagation can become fluid-like, rather than diffusive, and yields for graphite-based devices predictions in remarkable agreement with experiments [6]. References

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[6] S. Huberman et al., Science 364, 375 (2019).

Thursday, January 30. 11:00 – 11:50

Models of molecules that offer more than more Moore

Paul Low,* Masnun Naher, Daniel R. Harrison, Feng Jiang, Sara Sangtarash, Wenjing Hong, Colin J. Lambert

*University of Western Australia, AU

The field of molecular electronics has advanced rapidly following the development of convenient laboratory methods for the construction of electrode | molecule | electrode 'molecular junctions', and the use of these devices in the measurement of through-molecule conductance. These studies have allowed exploration of the electrical properties of a wide range of molecular structures, establishing a number of structure property relationships and leading to improved concepts for the design of molecular 'components' with high electrical conductivity, outstanding rectification ratios, and transistor-like gated conductance. In addition, uniquely molecular phenomena that influence the transmission of charge such as quantum interference (QI) have been identified providing new avenues for molecular design, and leading to proposals for the design of molecular materials with useful properties such as an enhanced thermoelectric figure of merit ZT and promisingly high power factors. Such concepts and associated investigations contribute to a growing awareness of the potential for molecular junctions to offer function beyond electron transport. However, whilst methods of measuring conductance have become more widely available, the technique remains relatively specialised. Alternatively, mixed valence models have a long history of use in modeling charge transfer processes predating metal|molecule|metal junction measurements. Spectral data, in the form of intervalence charge transfer (IVCT) bands, often found in the NIR-IR region, and characteristic IR spectroscopic markers are easily obtained and can be analysed using a variety of theoretical treatments. In this presentation we show evidence for the ability to control QI effects in both molecular junctions and mixed-valence models through the introduction of pendant groups to the periphery of 1,3-diethynyl benzene based systems. The potential to use spectroelectrochemical methods to rapidly screen target systems for QI as an aid to the further development of structure-property relationships in molecular electronics will be discussed.

Thursday, January 30. 11:50 – 12:10

Thermal and thermoelectric transport of OPE3 derivatives

Andrea Gemma,* H. Dekkiche, N. Mosso, S. Sangtarash, U. Drechsler, M. Calame, C. Lambert, M. R. Bryce, H. Sadeghi, and B. Gotsmann

*IBM Research Zurich, CH

Molecules have proved to be extraordinary platforms to test quantum transport mechanisms. Molecules are also expected to be tuneable towards high Seebeck coefficient and thermoelectric efficiency, due to the discreetness of their energy levels and the tunability of their characteristics via a precise control on the chemical synthesis. Those features make molecules interesting systems to be studied as thermoelectric converters or energy harvesting devices. Here we use a break-junction setup based on a Scanning Tunneling Microscope tip in contact with a gold-covered suspended platform, acting as high thermal insulated thermometer (>107 K/W) and high precision heat flux sensor (<10 pW). Electrical and thermal measurements through single molecules are shown, together with measurements of the thermoelectric power. A comparison between different oligo(phenylene ethynylene)(OPE3) derivatives with dithiol or di(dihydrobenzothiophene) anchor groups is given as well as a benchmarking with the smaller octanedithiol molecule. We show the quantization of the electrical conductance due to the availability of only a finite number of transport channels in the junction, the measurement of molecular thermal conductance with picowatt resolution and the Seebeck coefficient for molecules with the same electrical backbone but different side groups attached to the central ring of the OPE3 backbone. Our work develops a reliable method to characterize transport at the single molecule level and is a step towards the complete measurement of thermoelectric efficiency of molecular junctions.

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Acknowledgments: We acknowledge funding by the European Commission H2020-FETOPEN 'EFINED' (no 766853) and H2020-FETOPEN 'QuIET' (no 767187).

Thursday, January 30. 12:10 – 12:30

STM-based single-molecule thermopower: a comparative study

Joseph Hamill,* Tim Albrecht

*University of Birmingham, UK

We report a method using scanning tunneling microscope (STM) single molecular break junctions (SMBJ) to simultaneously measure the single molecular thermopower and electrical conductance of three test molecules, 1) oligo-phenylene ethynylene (OPE3), 2) octanedithiol (ODT), and 3) 4,4′-bipyridine (44BPY). The three measured Seebeck coefficients agree with literature values, with comparable or improved error. Good materials for thermoelectric applications must have high Seebeck coefficient, S, and high electrical conductivity, s, but must also have low thermal conductivity, k, summarized in the thermoelectric figure of merit, ZT. Recently it has been suggested that organic molecules may be tuned to yield high ZT and surpass even the best state-of-the-art thermoelectrics. Our reported method statistically correlates the Seebeck voltage offset, electrical conductance, and stretching displacement of the single molecular junction, introducing a powerful multivariate method for studying the interdependence of two important variables contributing to ZT. This method enables future exploratory work in single molecular thermoelectrics. Our method uses the variance measured during the measurement to correct for offsets in the electronics before calculating the voltage offset due to the single molecular thermopower, reducing the variance in the voltage offset to below 1 μV, yielding improved precision in the measured voltage offsets, and reducing error in our calculated Seebeck coefficients.

Thursday, January 30. 14:00 – 14:50

Room-temperature quantum effects in graphene nanogaps

Jaime Ferrer*

*Universidad de Oviedo, ES

Graphene has emerged in the past decade as a possible material of choice for nanojunction electrodes and/or transport channel. Diverse room-temperature quantum effects have been unveiled, that are a manifestation of the high mobility that electrons enjoy in this material. We will focus here on graphene break junctions, and show several examples of quantum interference effects and quantum dot physics

Thursday, January 30. 14:50 – 15:10

Rectification mechanisms in graphene three-terminal nanojunctions

Ivan Shorubalko,* P. Butti, K. Ensslin

*Swiss Federal Laboratories for Materials Science and Technology (Empa), CH

Recently, intrinsic voltage rectification in graphene three-terminal nanojunctions was demonstrated at room temperature [1]. The mechanisms influencing the efficiency of rectification are still not well understood. Finite element simulations (with COMSOL Multiphysics software package) are performed to model diffusive transport in the different geometries of the devices [2]. These field-effect simulations explain the observed rectification effect only partially. In our latest experiment we investigate the rectification effect in an exfoliated-graphene three-terminal nanojunction (100 nm constrictions) on Si/SiO2 at room temperature and 87 K [3]. Room-temperature rectification efficiency (ratio of output against input voltage) reaches 40%, which is higher than most efficiencies reported in the literature. The observed efficiency is higher at room temperature than at 87 K, which is in contrast to field-effect simulations and indicates that other mechanisms contribute to the rectification effect. We propose an explanation based on Joule heating and thermal voltages, as the device is operated in regimes of substantial power dissipation. Predicted thermal voltages show temperature, bias- and gate-voltage dependences which are similar as in our experiment. We conclude that Joule-heating effects need to be considered for GTTJ devices. Our work also suggests that multi-terminal nanojunctions can serve as an experimental playground to investigate thermo-electric effects in graphene at high temperatures, in constrictions, and at large thermal gradients.

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Thursday, January 30. 15:10 – 15:30

Phonon-engineered solids constructed from nanocrystals

Maximilian Jansen,* Nuri Yazdani, Vanessa Wood

*ETH Zürich, CH

The assembly of semiconductor nanocrystals (NCs) into conductive and ordered solids is of interest for a wide range of electronic applications. Control of the constituent NCs allows for a facile tuning of the NC solids electronic, structural and thermal properties. An important contributor to the thermal characteristics is the vibrational spectrum of the NC solid. We expect inter-particle vibrations, which are analogous to phonons on the atomic level, to be of importance for long range heat transport. These vibrational excitations involve multiple NCs and are of a longer length scale than any other vibration type in the NC solid. By implementing a three-dimensional mass-spring model, we demonstrate the behavior of these long-range vibrations as an effect of mass-spring disorder. Using the model we explore the parameter space of particle size and ligand type and their effect on the energy regime of the inter-particle vibrations. Additionally, we experimentally confirm their existence through inelastic neutron scattering and determine their characteristic energy scale and density. We successfully demonstrate that the energy regime of these inter-particle excitations can be engineered by varying particle size and ligand type of the NCs.

Thursday, January 30. 16:00 – 16:50

Assembly strategies for the fabrication of parallel individual arrays of single-molecule junctions with applications in molecular electronics and thermoelectric energy conversion.

Pilar Cea,* Lucia Herrer, Santiago Martín

*University of Zaragoza, ES

Molecular electronics, i.e. the use of molecules as single elements in circuitry opens the door to an exciting coming technology with high value-added electronic products including an increase in switching performance and faster processors, as well as a decrease in the energy consumption and then larger battery life of electronic products. Importantly, one of the most promised envisioned applications of molecular electronics is thermoelectrics, i.e., efficient conversion of (waste)-heat to electricity. Molecules acting as power converters could reuse the dissipation heat produced by (molecular) electronic devices into electricity to (partially) supply the power required to operate the device, which would be translated in a very low electronic power consumption. However, despite the enormous advances in this field several scientific and technological challenges should be surmounted before such a technology can be implemented in the market. In this context, integration of molecules to form densely integrated individually addressable arrays of multiple single-molecule devices in a parallel way is a major challenge, that also includes the fabrication of reliable, robust and uniform contacts between molecules and electrodes, the deposition of the second (top) contact electrode, and development of assembly strategies for precise placement of molecular materials within device structures. In this talk we will discuss advances in nanofabrication techniques used for the assembly of monomolecular films onto conducting or semiconducting substrates as well as recent methods developed for the deposition of the top contact electrode highlighting the advantages and limitations of the several approaches used so far. This contribution also aims to define areas of outstanding challenges in the nanofabrication of monomolecular layers sandwiched between two electrodes and opportunities for future research and applications.

Thursday, January 30. 16:50 – 17:10

From single molecules to ultra-thin layers: atomically precise molecular architectures for thermoelectrics

Samuel Jarvis*

*Lancaster University, UK

A key challenge in organic thermoelectric design and fabrication is to develop scalable and highly ordered ultra-thin layers whilst maintaining well defined single molecule properties. Self-assembly of single molecules provides an elegant solution to this problem, allowing a high degree of tunability when growing uniform molecular layers of, in principle, identical `single' molecules. Here I will discuss how surface science techniques in ultra-high vacuum (UHV) can address these challenges by exploiting UHV molecular growth and atomic resolution scanning probe microscopy (SPM). We show how pristine ordered molecular layers (e.g. C60 fullerene, porphyrin and OPE based molecules) grown in atomically clean environments can survive ambient conditions, without any loss in sample quality. Moreover, we show how UHV grown samples can be used as atomically precise base layers for further growth with solution-based self-assembly. I will discuss how methods initially pioneered to study single bond intra-[1] and inter-molecular[2,3] structure can be applied in ambient conditions, allowing us to completely characterise molecular ordering and uniformity with sub-nm resolution, and potentially identify key properties of single molecules within ordered films[4].

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Thursday, January 30. 17:10 – 17:30

Carbazole-Based Tetrapodal Anchor Groups for Gold Surfaces: Synthesis and Conductance Properties

Luke O'Driscoll,* Xintai Wang, Michael Jay, Andrei S. Batsanov, Hatef Sadeghi, Colin J. Lambert, Benjamin J. Robinson, Martin R. Bryce

*Durham University, UK

As the field of molecular-scale electronics matures and the prospect of devices incorporating molecular wires becomes more feasible, it is necessary to progress from the simple anchor groups used in fundamental conductance studies to more elaborate anchors designed with device stability in mind. This study presents a series of oligo(phenyleneethynylene) wires with one tetrapodal anchor and a phenyl or pyridyl head group. The new anchors are designed to bind strongly to gold surfaces without disrupting the conductance pathway of the wires. Conductive probe atomic force microscopy (cAFM) was used to determine the conductance of self-assembled monolayers (SAMs) of the wires in Au–SAM–Pt and Au–SAM–graphene junctions, from which the conductance per molecule was derived. For tolane-type wires, mean conductances per molecule of up to log(G/G0) = -4.37 (Pt) and log(G/G0) = -3.78 (graphene) were measured, despite limited electronic coupling to the Au electrode, demonstrating the potential of this approach. Computational studies of the surface binding geometry and transport properties rationalise and support the experimental results.

Friday, January 31. 09:00 – 09:50

Coherent population trapping by dark states formation in carbon nanotubes

Milena Grifoni,* Andrea Donarini, Michael Niklas, Michael Schafberger, Nicola Paradiso, Christoph Strunk

*University of Regensburg, DE

Illumination of atoms by resonant lasers can pump electrons into a coherent superposition of hyperfine levels which can no longer absorb the light. Such superposition is known as a dark state, because fluorescent light emission is then suppressed. Here we report an all-electric analogue of this destructive interference effect in a carbon nanotube quantum dot. The dark states are a coherent superposition of valley (angular momentum) states which are decoupled from either the drain or the source leads. Their emergence is visible in asymmetric current-voltage characteristics, with missing current steps and current suppression which depend on the polarity of the applied source-drain bias. Our results demonstrate coherent-population trapping by all-electric means in a macromolecular junction.

Nature Communications 10, 381 (2019)

Friday, January 31. 09:50 – 10:10

Pathways for the device integration of atomically precise Graphene nanoribbons

Oliver Braun,* Jan Overbeck, Gabriela Borin Barin, Mickael L. Perrin, Maria El Abbassi, Rimah Darawish, Qiang Sun, Guido Gandus, Roman Furrer, Pascal Ruffieux, Sara Sangtarash, Colin Lambert, Thorsten Prechtl, Akimitsu Narita, Klaus Müllen, Oliver Gröning, Kristjan Eimre, Edward Ditler, Colin Daniels, Vincent Meunier, Carlo A. Pignedoli, Hatef Sadeghi, Roman Fasel, Michel Calame

*Swiss Federal Laboratories for Materials Science and Technology (Empa), CH

Graphene nanoribbons (GNRs) have attracted considerable interest due to their largely modifiable electronic properties, including width-dependent bandgaps for armchair GNRs and spin-polarized edge states for GNRs with zigzag edges. Manifestation of these properties requires atomically precise GNRs which can be achieved through a bottom-up synthesis approach under ultrahigh vacuum conditions. We show that GNRs can be processed under ambient conditions and incorporated as the active material in a field effect transistor. At room temperature a film like behavior is observed while at cryogenic temperatures coulomb blockade and single electron tunneling can be seen. Our recent results may enable the realization of devices based on carbon nanomaterials with exotic quantum properties. The focus of this presentation will be on the integration of GNRs into devices and their transport properties.

Friday, January 31. 10:10 – 10:30

Relationship between Structure and Single-molecule Conductance and Thermoelectric Properties of Dipyridylfluorene Derivatives

Gunnar Olsen,* Gilles Yzambart, Laura Rincón-García, Iain Grace, Alexandros El Sachat, Colin J. Lambert, Nicolás Agraït, Martin R. Bryce

*Durham University, UK

Control of charge transport through single molecules is of fundamental interest in development of molecular electronic devices. The understanding hereof has benefitted immensely from well-designed structure/property studies. Advances in measuring techniques has opened up the field of single molecule thermoelectric, however only a few structure/property studies have been reported and our understanding of how to control thermoelectric properties is still in its infancy. We have synthesized a range of dipyridylfluorene derivatives with differing C9 functionality to elucidate the relationship between structure and thermoelectric properties at the single molecule level, especially thermopower. A modified scanning tunnelling microscope-break junction (STMBJ) technique was used to investigate the fluorene-series. As expected charge transport measurements showed no significant deviation in electrical conductance, however the systematic chemical modifications of the fluorine unit was observed to have a significant effect on the thermopower.

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Friday, January 31. 11:00 – 11:50

Charge Transport in Porphyrin Wires and Molecular Electronic Circuits

Harry Anderson*

*University of Oxford, UK

Porphyrins are large redox-active pi-systems, which makes them interesting components for the construction of molecular wires and transistors. This talk will summarize recent work on transport and charge delocalization through porphyrin monomers and large porphyrin arrays, such as butadiyne-linked nanorings. When edge-fused porphyrin tapes are connected to gold electrodes, their conductance is almost independent of length. Experimental results will also be presented from similar molecules connected across graphene nanogaps. Nanorings display aromatic and anti-aromatic ring currents in a range of oxidation states, which demonstrates that phase coherence is preserved over distances of more than 10 nm; the challenge is to exploit this quantum coherence in single molecule devices.

Friday, January 31. 11:50 – 12:10

Multipath OPE-based Molecules as Mechanically-Modulated Molecular Wires

Almudena Gallego,* Luca Ornago, Herre van der Zant, Marcel Mayor

*University of Basel, CH

A series of multipath OPE-based molecules have been proposed to investigate their thermoelectrical properties. The target molecules posse several electronic transport channels, which is predicted to be the origin of interference phenomena. The macrocycles are small enough to guarantee the efficient electronic conductivity and furthermore, their molecular design will allow for exploring the mechanical manipulation principle of quantum interference. In addition, the molecules are synthesized in two different configurations (pseudo-meta and pseudo-para) in order to study the influence of the electron pathway in the electronic performance.

Friday, January 31. 12:10 – 12:30

Thermoelectrical properties of self-assembled molecular-scale junctions

Benjamin Robinson*

*Lancaster University, UK

Molecular thin films, such as self-assembled monolayers (SAMs), offer the possibility of translating the optimized thermophysical and electrical properties of high-Seebeck-coefficient single molecules to scalable device architectures. Here I will report on our recent progress in the design, fabrication and characterisation of thermoelectric SAMs. This includes a new reproducible and non-destructive method for probing the electrical and thermoelectric properties of small assemblies (10 – 1000) of thiol-terminated molecules arranged within a SAM on gold and demonstrate the successful retention of the single-molecule electrical conductivity and Seebeck values. We have used a modified thermal-electric force microscopy approach, which integrates the conductive-probe atomic force microscope with a sample positioned on a temperature controlled heater, operating with a probe-sample peak-force feedback that interactively limits the normal force across the molecular junctions. We have begun with well-understood molecular structures such as alkanes and biphenylthiol to benchmark our electrical and Seebeck coefficient measurements before exploring more complex anthracene-based molecules which demonstrate significant quantum interference effects at room temperature. We have also explored the thermoelectric effects of well-defined layers of pi-pi stacked tetraphenyl porphyrins where we observe that the Seebeck coefficient showed a strong dependency from film-thickness resulting in an enhanced value of 72 μV/K at ~5nm thickness (compared to ~15 μV/K for the monolayer film). The experimental results are fully supported by density functional theory calculations of the thermal and electrical quantum transport properties of single and small clusters of molecules.

Poster abstracts

Listed in alphabetical order according to the last name of the first author.

Controlling Fano Resonances in Carbene-Metal-Amides

Abdelkareem Almeshal*

*Lancaster University, UK

We identify Fano resonances in the transport properties of carbine-metal amides and demonstrate that their energetic location and magnitude can be controlled by varying the connectivity of the core to external electrodes and by rotating the pendant moiety connected to the current-carrying core. The Fano resonances can be suppressed by rotating the pendant group and increasing the linkages to electrodes.

Tuning the electrical properties and thermal power by manipulating the connectivity in thiophene-diketo-pyrrolopyrrole (DPP) derivatives

Renad Almughathawi,*

*Lancaster University, UK

Manipulating the connectivity of external electrodes to central rings of carbon-based molecules is a novel route to tuning the electrical and thermoelectrical properties of single molecules. Here we investigate the connectivity dependence of a series of thiophene-DPP molecules using density functional theory combined with tight binding models. First, we investigated charge transport through gold/thiophene-DPP/gold hybrid junctions and found a significant dependence of electrical conductance on the connectivity of the two thiophene rings on both side of DPP core. In addition, we further looked into the thermopower of the derivatives and demonstrated that the connectivity of five-member ring could increase the thermopower and even change its sign. The origin of this connectivity effect is clarified using both DFT and TB models. We also found the electrical and thermal properties are sensitive to the angle between –SCH3, gold and backbone of molecule.

Constructive Quantum Interference in Anthracene Core

Ahmad Abdulrhman Almutlg,* Ali Ismael, Colin Lambert

*Lancaster University, UK

A key area of activity in contemporary molecular electronics is the control of quantum interference (QI) in molecular junctions and devices. A range of strategies have been employed to understand and regulate QI, with features such as chemical substitution, aromaticity and conjugation, electrochemical potential, non-covalent interactions being varied and connectivity. Magic ratio rules (MRR) have been developed to predict QI patterns in polycyclic aromatic hydrocarbons. MRRs have been successful in explaining observed electronic transport properties of molecular junctions. This study tests the validity of magic ratio rules in fully conjugated anthracene core with two different connectivities 7,2′ and 1,5′ and two anchor groups including thioacetate and thioether.

Breakdown of Curly Arrow Rules in Anthraquinone

Jehqan Alqahtani,* Hatef Sadeghi, Sara Sangtarash, Colin J. Lambert

*Lancaster University, UK

Understanding and controlling quantum interference QI in single molecules is fundamental to the development of QI based single molecule electronics. Over the past decade, simple rules such as counting rules, curly arrow rules, circuit rules and more recently magic ratio rules have been developed to predict QI patterns in polycyclic aromatic hydrocarbons. These rules have been successful in explaining observed electronic transport properties of molecular junctions and provide helpful design tools for predicting properties of molecules before their synthesis. Curly arrow rules are widely used by chemists, material scientists and physicists to predict destructive QI. Here we examine the validity of curly arrow rules in fully conjugated anthracene and dihydroxyanthracene, cross-conjugated anthraquinone and broken conjugated dihydroanthracene attached to graphene or gold electrodes through pi-pi stacking or thiol and Au-C anchors. For the first time, we demonstrate that curly arrow rules break down in molecular junctions formed by cross-conjugated anthraquinone. In contrast with the destructive QI predicted by curly arrow rules for a meta connected anthraquinone core, we demonstrate that QI is constructive. This behavior is independent of the choice of electrode material or anchor groups. This is significant, because by changing the redox state of meta connected dihydroxyanthracene to form meta connected anthraquinone, the conductance of the junction increases by couple of orders of magnitude due to the cross over form constructive to destructive QI. This opens new avenues for realization of quantum interference based single molecule switches.

Constructive Quantum Interference in single-molecule junctions

Majed Alshammari,* Ali Ismael, Colin Lambert

*Lancaster University, UK

A key area of activity in contemporary molecular electronics is the control of quantum interference (QI) in molecular junctions and devices. A range of strategies have been employed to understand and regulate QI, with features such as chemical substitution, aromaticity and conjugation, electrochemical potential, non-covalent interactions and connectivity. Magic ratio rules (MRR)[1] have been developed to predict QI patterns in polycyclic aromatic hydrocarbons. MRR have been successful in explaining observed electronic transport properties of molecular junctions. This study tests the validity of magic ratio rules in fully conjugated anthracene cores when they are combined in series with either a graphene sheet or a planar porphyrin molecule.

Electron transport in tethered pi-stacked junctions formed from carbazoles

Noorah Alwhaibi*

*Lancaster University, UK

Studying charge transfer through π stacked molecules has opened up new challenges in the single molecule level. In this work we introduce a way of controlling the stacking geometries of Carbazole molecules by tethering them with different lengths of alkyl chain, and study the transport properties of these molecules. Using a combination of density functional theory and the quantum transport code GOLLUM we calculate the electronic transport and the conductance of these systems. The results demonstrate that a closed hairpin structure is the most favourable one. Furthermore, we found that the conductance and the geometries are roughly independent of the length of the tether.

Molecular thermoelectrics: from single molecules to SAMs

Sophie Au-Yong,* Leonardo Forcieri, Xintai Wang, Benjamin J. Robinson, Samuel P. Jarvis

*Lancaster University, UK

Optimising electricity generation from thermoelectric devices requires maximising the Seebeck coefficient and the thermoelectric figure of merit. Single molecules are a promising way to achieve this goal, as quantum interference effects can be exploited to optimise transport [1]. Transport properties can be tuned using different molecules with specific interactions, making them ideal for thermoelectric applications. Whilst single molecule behaviour is well understood, there are enormous challenges scaling this up to a full device, as even small numbers of defects can cause significant deviation from the predicted high efficiencies, and so suitable techniques must be determined. In this study we discuss fabrication of molecular films consisting of molecules which complex via metal coordination. We combine two techniques, thermal sublimation in ultra-high vacuum (UHV) and solution self-assembly, each characterised with submolecular resolution atomic force microscopy (AFM) [2] and x-ray photoelectron spectroscopy (XPS). We discuss the challenges with these materials, and the delicate balance between surface-molecule, molecule-molecule and molecule-solvent interactions, which can be fine-tuned through molecular design.

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Anti-resonance features of destructive quantum interference in single-molecule thiophene junctions achieved by electrochemical gating

Abdalghani Daaoub*

*Lancaster University

Gating of quantum interference (QI) in the charge transport through single-molecule junctions is a crucial step towards novel functional molecular devices. In this work, we electrochemically manipulate the destructive quantum interference (DQI) in thiophene - based molecular junctions. we have employed electrochemical gating for the fine-tuning of charge transport properties in single-molecule thiophene junctions with and without. Benefiting from the high gating efficiency of electrochemical gating and the large potential windows of ionic liquid, this work provides the theoretical and experimental observation of charge transport at an anti-resonance state arising from DQI at room temperature. It is found that the gating of single- molecule thiophene junctions with DQI when the Fermi level is located between a resonance and anti-resonance. The electrochemical tuning of DQI presented in this work provides a promising design strategy for tuning of interference in future molecular materials and devices.

Synthesis of new OPE derivatives and a study of their electro-thermal properties in molecular junctions

Hervé Dekkiche,* Andrea Gemma, Fatemeh Tabatabaei, Samy Merabia, Thomas Niehaus, Bernd Gotsmann, Martin R. Bryce

*Durham University, UK

In the past few years, the development of new devices involving electronic technology have not ceased to increase both in demand and in complexity. With the miniaturization needed to build always smaller computers, smartphones and other tools that came along, new problems arose. Among them, the increase of the heating/power ratio represents one of the biggest issues.[1] The understanding of how electrons, photons and phonons interact together is not very well understood as yet. The work presented here is focused on investigating the phenomenon involved at the molecular level. We aim to study the single-molecule electro-thermal conductance of synthetically tailor-made chemical species anchored between the gold electrodes of a custom STM setup. To achieve that, several monomeric or oligomeric dihydrobenzothiphene-based oligophenylene-ethynylene (OPE) have been synthesized and studied.[2] The experimental results obtained are supplemented with computer simulations which use DFT principles.

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Quantum interference-induced conductance variation in mechanosensitive single-molecule junction

Chunwei Hsu,* Almudena Gallego, Maxim Skripnik, Marcel Mayor, Fabian Pauly, Herre van der Zant

*Kavli Institute of Nanoscience, Delft University of Technology, NL

A great interest of molecular electronics comes from its change in electronic structure through external stimuli, which provides functionality at the single-molecule level. Mechanically-controlled break junction (MCBJ) is a great tool for characterizing molecular properties and their response to different stimuli including light, solvent and importantly, mechanical deformation. In our recent MCBJ experiment, we showed that the conductance of [2.2] Paracyclophane-based molecular systems can be mechanically tuned up to an order of magnitude at room temperature. The physical origin of such feature is a consequence of destructive quantum interference between the frontier orbitals. This indicates not only a possible application for mechanical sensors based on this class of molecules, but also show an example of mechanically-tuned quantum interference. Following this intriguing result, we investigate other properties of this molecule, such as I-V characteristics at low temperature. We are also exploring other molecules with similar spring-like structures, where quantum interference effect is expected to manifest.

Conductance and Thermopower of Cross Conjugated Carbazoles

Juan Hurtado-Gallego,* Laura Rincón-García, Nicolás Agraït

*Universidad Autónoma de Madrid, ES

We have studied the conductance and Seebeck coefficient of molecular junctions of three different cross conjugated carbazoles using the STM break junction technique. The conductance and thermopower are measured simultaneously using a modified STM as the molecular junction is stretched. Each molecule shows two different values of conductance and Seebeck coefficient, in the range of $10^{-3.5}$ to 10^{-5} G/G0 and -8 to -14 μV/K respectively. We also observe two different types of IV curves, sharper for the higher conductance values and flatter for the lower ones.

Conductance and Thermopower of Blatter Radicals

Juan Hurtado-Gallego,* Laura Rincón-García, Nicolás Agraït

*Universidad Autónoma de Madrid, ES

We have studied the conductance and Seebeck coefficient of molecular junctions of three different Blatter Radicals using the STM break junction technique. The conductance and thermopower are measured simultaneously using a modified STM as the molecular junction is stretched. Organic radicals are open-shell systems containing one unpaired electron, which makes them potentially interesting for thermoelectric applications. In each molecule we find several distinct conductance plateau values ranging from 10^{-2} to 10^{-5} G/G0 while the Seebeck coefficients are rather independent of the conductance for each of the radicals with values from -9.4 μV/K to a relatively high value of -24.6 μV/K.

Characterization of a novel thermal sensor for STM-based thermal conductance measurements

Rubén López Nebreda,* Juan Jose Velasco, Laura Rincón-García, Nicolás Agraït

*Universidad Autónoma de Madrid, ES

We have manufactured and characterized a hot wire based thermal probe based on 5µm diameter Wollaston wires. Using this probe as a STM tip will allow us to explore the thermal conductance of atomic contacts. To characterize the thermal behaviour of the probe, we heat the wire with an AC current, which allows us to use lock-in detection to measure the resistance of the wire thereby determining very precisely variations of the average temperature of the wire. We study the evolution of the temperature as the distance from the substrate is varied in ambient conditions. Comparison with a theoretical model based in finite differences and including the effect of convection yields a detailed understanding of the thermal behaviour of the probe and provides an accurate calibration of its sensitivity.

Acene substituted OPE3s: a platform for comparing single-molecule conductance measurement techniques

Luca Ornago,* Yuru Liu, Alfredo Rates, Marco Carlotti, Maria El Abbassi, Ryan C. Chiechi, Herre S.J. van der Zant

*Kavli Institute of Nanoscience, Delft University of Technology, NL

Over the years, several techniques have been developed for the measurement of the electronic properties of molecules, both for self-assembled monolayers and at the single-molecule level [1]. Among these, break-junction based techniques have gained interest for their statistical robustness, which allows for electronic characterization of a single molecule at room temperature. This work focuses on the comparison of scanning tunneling microscope (STM-BJ), mechanically controllable break-junctions (MCBJ), as well as molecular ensemble techniques, using a series of oligo(phenylene-ethynylene) (OPE3) derivatives. Due to their simple structure, and well understood properties, this class of molecules represents an ideal platform to benchmark and compare the results obtainable through the different approaches. By substituting the central phenyl ring of OPE3 with acenes of increasing length, the chemical moieties were designed to have increasing p- p stacking strength, allowing to investigate the effect on the low conductance features that arise from such interactions [2]. Additionally, an unsupervised clustering algorithm has been employed to gain further insight on the extracted single molecule conductance values and their correlation to the molecular structure [3].

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Compact [2.2]Paracyclophane (PC)-based systems

Ksenia Reznikova,* Almudena Gallego, Chunwei Hsu, Herre van der Zant, Marcel Mayor

*University of Basel, CH

Recently, molecular electronics have attracted great interest. The measurement of conductance through single molecules, using the mechanically controlled break junction technique (MCBJ) is performed on a plethora of structures. Here, we focus on [2.2]paracyclophane (PC), a prototypical, layered hydrocarbon with two benzene rings in a face to face orientation. PC has several unique properties such as through-space conjugation and formation of pseudo-geminal electrophilic substitution. Motivated by previous results studying the electrical and mechanical behavior in a pseudo-para [2.2]paracyclophane system, we have synthesized a library of more compact structures with a pseudo-para and pseudo-meta core and thio-acetyl anchoring groups in para and meta positions. The synthesis of next-generation molecules has an even more compact and highly conjugated system which is based on a naphthalene[2.2]paracyclophane.

Tailor-Made Molecular Rods for Graphene Junctions

Ksenia Reznikova,* Lorenzo Delarue Bizzini, Markus Neuburger; Asela Christy, Daniel Häussinger, Maria El Abbassi, Oliver Schmuck, Michel Calame, Marcel Mayor

*University of Basel, CH

Graphene has been applied in several technologies since its discovery in 2004. A new promising idea is to use graphene as a contact material in nanoelectronics. For this application, graphene is superior to gold because of its stability, 2D structure and large variety of possible anchoring groups. Here, we will present the synthesis and further studies on a series of tailor-made molecular rods for graphene junctions. The desired molecules are designed to bridge a nanogap between two graphene electrodes on a silicon insulator. The molecular rod consists of a central moiety that is modified with two silica anchoring groups to prevent the molecular rod from sliding out of the junction. Oligo(phenylene-ethynylene) (OPE) linkers establish the electronical communication and outer aromatic anchoring groups contact graphene via p-p interactions. We propose the synthesis of a library of OPEs with different lengths, containing various aromatic groups for the deposition to the graphene surface.

Electrical contacting of molecules for thermoelectricity

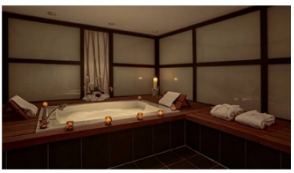
Oliver Schmuck,* Oliver Braun, Mickael Perrin, Davide Beretta, Michel Calame

*Swiss Federal Laboratories for Materials Science and Technology (Empa), CH

Single molecules are promising organic semiconductors for the purpose to increase the efficiency of thermoelectric devices at the nanoscale. To be able to porbe the electrical and thermoelectric properties of these molecular junctions the molecules need to be contacted. Here we present an approach to contact single molecules in graphene based junctions to probe their electrical transport properties and measure the thermoelectric effects. The devices fabricated are based on graphene field effect transistors with nanometer sized gaps in the graphene to contact the single molecules. The molecules can either bridge the graphene gap or form a molecular stack consisting of several molecules. A second approach is to form networks of molecular junctions via gold nanoparticle arrays and exchange the ligand molecules between the single particles to probe the electrical and thermoelectric properties of the film formed.

The Venue





The conference will take place at the H+ Hotel & SPA Engelberg at the foot of the Titlis Massif, in the center of Engelberg, at an elevation of 1000 meters. The hotel is provided with a wellness area, where to unwind and switch off after a long day or treat yourself to a massage. The 200 square meter spa area includes an indoor pool, a Finnish sauna, and aromatic steam room, experience showers and an ice grotto. All rooms are non-smoking and provided with high-speed internet (Wi-Fi). Each guest will receive a password to freely access internet during the entire period of the conference.

More information about the venue can be found at the website of the hotel.

NOTE: if you plan to extend your stay before or after the conference, please contact the Hotel directly to arrange your stay.

How to reach the conference site

By train

All participants are recommended to travel to Lucerne, where to board the Luzern-Engelberg Express that reach the town of Engelberg in only 43 minutes. The H+ Hotel is only a four minutes walk away from the train station (see map). Please consult the Swiss Federal Railway (SBB) website or download the SBB mobile app to plan your trip.

By plane

Travellers are recommended to fly to Zurich International Airport or Basel International Airport, and from there to reach the town of Engelberg by train. Engelberg train station is approximately 2 hours away form Zurich International Airport and 2h 30min away from Basel International airport. The H+ Hotel is only a four minutes walk away from the train station (see map). Please consult the Swiss Federal Railway (SBB) website or download the SBB mobile app to plan your trip.

Quick facts about Engelberg

Here follows a list of information that you might find useful to facilitate and better enjoy your stay in Engelberg.

Mobility: busses within Engelberg are free of charge.

For ski lovers: ski passes can be purchased at the reception of the hotel, and reductions are available for groups of minimum 10 people.

For cheese lovers: Switzerland's only publically accessible artisan cheesemaking production within a monastery is in Engelberg. There you can watch cheese being hand-produced and regional milk being crafted into specialities, such as the famous "Engelberger Klosterglocke" from 10:00 am to 3:00 pm daily. The venue offers entertaining and informative demonstrations, covering a variety of topics - all to do with cheese. For more information, visit the website. Reservation might be necessary.

For coffee lovers: the Roastery on Dorfstrasse 9 is the small and relaxed heart of all operations. It is the place where to roast, package and prepare for deliveries. In the afternoon the doors are open to the shop and coffee bar. For more information, visit the website. Reservation might be necessary.

Information about events in Engelberg can be found at the official website of Engelberg's Tourist Office. Reductions for Engelberg's sights might be available with guest cards (issued by the hotel). Please ask directly at the hotel's reception for more information.