

# Gathering on Transport at the Nanoscale

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- 46. Philipp Stegmann -- University Duisburg-Essen
- 47. Thijs Stuyver -- University of Brussels
- 48. Nikodem Szpak -- University Duisburg-Essen
- 49. Manan Vyas -- Universidad Nacional Autónoma de México
- 50. Dietrich Wolf -- University Duisburg-Essen

#### Talk 1: Monday 10:00-11:00

#### Electronic transport and conversion processes in molecular materials: a multiscale challenge for electronic structure theory

Björn Baumeier -- Eindhoven University of Technology

Functionality of molecular devices, such as organic solar cells or light emitting diodes, is determined by the dynamics of electronic excitations and conversion processes within multilayered structures. Typically processed from solution, the material morphology in the functional layers and at their interfaces is characterized by a substantial amount of structural disorder, which is further amplified by thermal disorder at room temperature operating conditions.

This situation constitutes an enormous challenge for an ab-initio modeling of dynamical processes in such materials. In my presentation, I will introduce our multiscale approach, which combines Molecular Dynamics, electron transfer theories, excited state electronic structure methods in QM/ MM setups, and rate-based dynamics. Within this framework, I will specifically discuss the effects of including many-body corrections to DFT within the GW-BSE approach, the influence of an explicit molecular environment on the obtained electronic excitations in theoretical spectroscopy, as well as singlet and triplet exciton diffusion.

#### Talk 2: Monday 11:30-12:30

#### Diradical Character as a Guiding Principle for the Insightful Design of Molecular Nanowires with an Increasing Conductance with Length

Thijs Stuyver -- University of Brussels, Hebrew University in Jerusalem

In recent years, a considerable interest has grown in the design of molecular nanowires with an increasing conductance with length. The development of such nanowires is highly desirable since they could play an important role in future molecular-scale circuitry. Whereas the first experimental observation of this non-classical behaviour still has to be realized, a growing number of candidate wires have been proposed theoretically. In the present contribution, we point out that all the wires with an "anti-Ohmic" increasing conductance with length proposed so far share a common characteristic: their diradical character increases with length. The conceptual connection between diradical character and conductance enables a systematic design of such anti-Ohmic wires and explains the difficulty in their syntheses. A strategy is proposed to balance the stability and conductance, so that this non-classical phenomenon can be observed.

#### Talk 3: Monday 12:30-13:30

# The kernel polynomial method for spintronics and quantum transport: Toward quantum simulation of macroscopic devices.

Jose Hugo García -- Institut Català de Nanociència i Nanotecnologia (ICN2)

#### Talk 4: Monday 15:00-16:00

#### Electronic structure of organic molecules and ligand-protected metal clusters: A first step toward the understanding of their conductive behavior

Ignacio L. Garzón Instituto de Física Universidad Nacional Autónoma de México 04530 CDMX, México garzon@fisica.unam.mx

Electron transport at the nanoscale is not only of fundamental interest in nanoscience due to the possible existence of unexpected and novel mechanisms of electron conduction through molecules and nanostructures, but also because of its potential applications in the fabrication of new devices useful for nanoelectronics. From a theoretical point of view, before such electron transport mechanisms can be investigated, it is necessary to select molecules and nanosystems with appropriate physicochemical properties such as their geometric and electronic structure. In this work, we theoretically investigated, by using first-principles (based on density functional theory) methods, the electronic structure of two promising nanomaterials that might display interesting electron conduction properties. One of them corresponds to a 2-D infinite array of ligand-protected Au nanoparticles possibly functionalized by dithiolated conjugated molecules: benzene-dimethanethiol (BDMT) and benzenedicarbonthialdehyde (BDCT). It is found that the non-functionalized lattices are insulating, with negligible band dispersions even for a compression of 20% of the lattice constant. Distinct behaviors of the dispersion of the lowest conduction band as a function of compression are predicted for the functionalized lattices: The band dispersion of the BDMT-functionalized lattice increases considerable with compression, while that of the BCMT-functionalized lattice decreases. [1] The second nanomaterial investigated corresponds to the all-trans polyacetylene molecule in neutral, cationic, and anionic states, with different chain length and under the influence of an external electric field. Here, we analyze the variation of the HOMO-LUMO gap and the appearance of electron localization as a function of the chain length, electric field, and charge state. The electronic structure results obtained for the abovementioned nanomaterials are expected to be useful as an initial step to investigate electron transport mechanisms at the nanoscale.

#### Talk 5: Monday 16:30-17:00

#### Phenomenological approach to transport through threeterminal disordered wires

Angel Martinez Argüello -- Benemérita Universidad Autónoma de Puebla

We study the voltage drop along three-terminal disordered wires in all transport regimes, from the ballistic to the localized regime. The system consists of a horizontal disordered wire connected to sources of voltage by one-open-mode perfect conductors on each terminal and a third terminal that measures the voltage drop along the horizontal wire, in an asymmetric configuration. We use two models to describe the disordered wire: The one-dimensional Anderson model with diagonal disorder and finite-width bulk-disordered waveguides. Our analysis is based on the voltage distribution of asymmetric three-terminal chaotic devices, depending only on the Dyson symmetry index  $\beta$ , valid for the three symmetry classes of random matrix theory: orthogonal, unitary and symplectic;  $\beta = 1, 2$  and 4, respectively. This distribution is extended to every continuous  $\beta > 0$  and used as a phenomenological expression. We show that it encompasses all the transport regimes where  $\beta$  shows a quadratic behavior as a function of the disorder strength.

#### Talk 6: Monday 17:00-17:30

Gathering on Transport at the Nanoscale

29 October - 9 November 2018 Centro Internacional de Ciencias Cuernavaca, México

#### **Resonant thermoelectric transport in DNA-like systems**

J. E. González<sup>1</sup> and Chumin Wang<sup>2</sup>

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The study the thermoelectric properties of DNA molecules, can be achieve by semi-empirical approaches, for electronic properties one of the most used is the so-called fishbone model [1]. Such model considers hopping integrals t of  $\pi$ -electrons between nearest-neighbor base pairs as well as between the nucleobase and sugarphosphate backbone represented as Fano defects. The semiconducting behavior of DNA molecules is used for thermoelectric applications [2]. Recently, neglecting the phonon contribution, a giant thermoelectric figure of merit by electrons (ZTel) induced by the sugar-phosphate backbones in a finite two-dimensional (2D) poly(G)-poly(C) DNA chain was predicted [3].



In this work, we present a full semi-empirical calculation of thermoelectric properties of macroscopic length DNA molecules that includes the phonon participation through a 2D coarse grain model of two sites per nucleotide [4]. Our two-site coarse-grain model, consists of one site representing the nucleobase that could be guanine, cytosine, adenine or thymine, and the other symbolizing the sugar-phosphate molecule. The interaction between these two sites are modeled by central and non-central restoring force constants, which were calculated from DNA longitudinal and transversal sound velocities estimated by the inelastic X-ray scattering. We found an enhanced thermoelectric figure-of-merit (ZT) in self-assembled DNA-like systems by using a real-space renormalization method developed for the Kubo-Greenwood formula, in which tight-binding and Born models are respectively used for the electric and lattice thermal conductivities. The results reveal that the quasiperiodicity could be another ZT-improving factor, whose long-range disorder inhibits low-frequency acoustic phonons insensitive to local defects [5]. This work has been partially supported by CONACyT-252943 and UNAM-IN113714. Computations were performed at Miztli of DGTIC, UNAM.

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#### Talk 7: Tuesday 10:00-11:00

#### Electron-phonon effects and signals in transport: From molecules to graphene

M. Brandbyge Technical University of Denmark, DTU Nanotech, Kgs. Lyngby, Denmark Center for Nanostructured Graphene (CNG)

In the Landauer approach electrons are assumed to bypass a nano-scale conductor ballistically, and equilibrate through energy exchange inside the bulk electrodes. However, when passing through the conductor the current-carrying electrons has a finite, albeit typically small, probability to interact with the atomic vibrations (phonons) in the device, leading to local energy and momentum transfer to the ions.

This electron-phonon interaction give rise to small signals in the current at low bias, corresponding to the vibrational energies in the junction. These signals can probe the atomic and electronic structure, and the interactions, inelastic electron transport spectroscopy (IETS). I will show how first principles calculations of IETS of molecules and graphene compares to experiments and what we can learn from the comparison [1,2,3].

In the presence of a high current density the electron-phonon interaction will not only lead to Joule heating: A number of other mechanisms have been pointed out in which the current may excite and influence the atomic motion in nano-junctions, and possibly lead to instabilities and atomic restructuring [4,5]. I will present methods and calculations to investigate the effects in atomic, molecular, and graphene-based junctions.

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#### Talk 8: Tuesday 11:30-12:30

# Full counting statistics of electron transport in nanoscale systems

Philipp Stegmann -- University of Duisburg-Essen

Transport of electrons though nanoscale systems such as quantum dots or metallic islands is a stochastic process determined, for instance, by the probabilistic nature of tunneling or a randomly changing environment. The number of the transferred electrons per time interval can be characterized by a probability distribution also referred to as the full counting statistics. Remarkable progress in nanotechnology has led to the development of electrometers so sensitive that transport of individual electrons can be observed in a time-resolved manner. Therefore, the probability distribution can be directly measured. However, it is quite challenging to analyze the information contained in the distribution. In my talk, I will elaborate on the benefits of factorial cumulants [1,2,3] as a tool to obtain useful information from the probability distribution.

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[2] E. Kleinherbers, P. Stegmann, and J. König, NJP 20, 073023 (2018).

[3] P. Stegmann, J. König, and S. Weiss, PRB 98, 035409 (2018).

#### Talk 9: Tuesday 12:30-13:00

## From the Dirac oscillator to the graphene strips, microwave experiments

John Alexander Franco

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For a long time analogous experiments have encouraged the development of a particular field, this was the case of quantum chaos [1], for example, where the phenomena predicted by the quantum billiards theory, unreachable at their time, were observed and extended by analogous experiments in microwave billiards. Today new milestones have been reached with this type of experiments, among which the only known experimental realization of the Dirac oscillator [2] proposed by Marcos Moshinsky almost 30 years ago. In this talk, we will deal with an updated overview of the experimental realizations with microwave analogs, some of their most recent achievements [3,4] and how these experiments have influenced the ideas established in the different fields of application.

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#### Talk 10: Tuesday 13:00-13:30

## From Klein to anti-Klein tunneling in graphene tuning the Rashba spin-orbit interaction or the bilayer coupling

Parisa Majari -- University of Kurdistan

The spin-orbit coupling is believed to play an important role in 2D insulators and it is important for the understanding of many physical effects. Rashba and intrinsic spin-orbit coupling are two types of spin-orbit coupling in graphene. The moving of electrons in the atomic electric field produce a magnetic field which interacts with the electron spin. So, graphene has a weak intrinsic spin-orbit coupling. However, the extrinsic Rashba spin-orbit coupling term arises due to an external electric field perpendicular to the graphene. We evaluate the transmission coefficient for a particle crossing a potential barrier in monolayer graphene with Rashba spin-orbit coupling and in bilayer graphene. We show that in both the cases one can go from Klein tunneling regime, characterized by perfect normal transmission, to anti-Klein tunneling regime, with perfect normal reflection, by tuning the Rashba spin-orbit coupling for a monolayer or the interplane coupling for a bilayer graphene. In addition, we present analytical results for the transmission dependence as a function of the direction of the incident electron and width of the barrier.

#### Talk 11: Tuesday 15:00-16:00

#### Valley engineering by strain in Kekulé-distorted graphene

Elías Andrade, Ramon Carrillo-Bastos, Facultad de Ciencias, Universidad Autónoma de Baja California, Apdo. Postal 1880, 22800 Ensenada, Baja California, México.

Gerardo G. Naumis

Depto. de Sistemas Complejos, Instituto de Física, Universidad Nacional Autónoma de México (UNAM). Apdo. Postal 20-364, 01000 México D.F., México

A Kekulé bond texture in graphene modifies the electronic band structure by folding the Brillouin zone and bringing the two inequivalent Dirac points to the center. This can result, in the opening of a gap (Kek-O) or the locking of the valley degree of freedom with the direction of motion (Kek-Y). We analyze the effects of uniaxial strain on the band structure of Kekulé-distorted graphene for both textures. Using a tight-binding approach, we introduce strain by considering the hopping renormalization and corresponding geometrical modifications of the Brillouin zone. We numerically evaluate the dispersion relation and present analytical expressions for the low-energy limit. Our results indicate the emergence of a Zeeman-like term due to the coupling of the pseudospin with the pseudomagnetic strain potential which separates the valleys by moving them in opposite directions away from the center of the Brillouin zone. For the Kek-O phase, this results in a competition between the Kekulé parameter that opens a gap and the magnitude of strain which closes it. While for the Kek-Y phase, in a superposition of two shifted Dirac cones. As the Dirac cones are much closer in the supperlattice reciprocal space that in pristine graphene, we propose strain as a control parameter for intervalley scattering.

#### Talk 12: Tuesday 16:30-17:30

#### Transmission of Anomalously and Anderson-Localized Waves and Intensity Inside Random Media

Victor Gopar -- University of Zaragoza

The presence of sources of disorder are ubiquitous in real materials and their effects on transport of classical and matter waves (EM & electrons, for instance) have been widely study. It is generally believed that disorder in 1D systems leads to an exponential spatial localization of waves, i.e., Anderson localization. Here, however, we present a model of disorder that induces anomalous localization of waves, or delocalization. Following that model (Lévy disorder), we provide experimental evidence demonstrating that anomalous localization of electromagnetic waves can be induced in microwave waveguides with dielectric slabs randomly placed following a Lévy distribution. This model is also applied to study anomalous localization of electrons in graphene nanoribbons.

To gain more insight the phenomena of complex scattering of wave, we also study some statistical properties of intensity of waves inside random media. Experimental data of microwave waveguides support our theoretical results.

#### Talk 13: Wednesday 10:00-11:00

#### Pathways in molecular conductance and spin coupling

#### **Carmen Herrmann**<sup>1</sup>

<sup>1</sup>Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, 20146 Erlangen, Germany

For understanding spin-polarized electron transport through molecular bridges and (exchange) spin coupling between local spin centers within in a molecule, it is interesting to know which parts of the molecule are responsible for mediating transport or spin interactions.

In the case of spin coupling, ferro- and antiferromagnetic pathways may add up or partially cancel, which is hidden if only the total spin coupling is considered. A new approach to decomposing spin coupling based on Green's functions [1] allows not only identifying which molecular parts are responsible for spin coupling in isolated molecules, but may also allow for distinguishing, e.g., between intramolecular and through-surface contributions [2].

In electron transport through molecular junctions, local decomposition of electron transmission will be used to highlight the importance of spin-polarized parts of the molecule for transport [3-7].

In both cases, the tunability of pathways by changes in the chemical structure will be discussed.



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## Talk 14: Wednesday 11:30-12:30

# Centrosymmetry, current vortices and energy distribution functions

Thomas Stegmann -- Universidad Nacional Autónoma de México

## Talk 15: Wednesday 12:30-12:45

#### **Electron Optics in Graphene Heterojunctions**

Elizabeth Mendoza & Emmanuel Paredes Universidad Nacional Autónoma de México

#### Talk 16: Wednesday 12:45-13:00

#### Partial positive refraction in asymmetric Veselago lenses of uniaxially strained graphene

Y. Betancur-Ocampo -- Universidad Nacional Autónoma de México

Asymmetric Veselago lenses (AVLs) can be created from ballistic p-n and np-n homojunctions of uniaxially strained graphene. This atypical converging electron flow emerges by applying uniaxial tension out of the device's symmetry axes. A part of electron flow needs to be positively refracted for focusing in an asymmetric spot, whose location is tunable with the strain. In AVLs, Klein tunneling is angularly shifted regards to the normal incidence. This perfect transmission occurs at the straight line that connects the point source and focus, which is unaffected by variation of the Fermi level and voltage gate. Moreover, the mirror symmetry breaking

by the strain also causes the asymmetry in Fabry-Perot interference. The novel electron optical laws allow to evidence that reflected and refracted electrons in AVLs lie on the same straight line with opposite group velocities and pseudo-spins. Unlike isotropic graphene, electrons under normal incidence present backscattering, angles of reflection and refraction different to zero. The average particle transmission is higher (lower) than isotropic case when the tensile strain is increased near (far away) the normal direction. These results may be useful for designing strain-bendable probing tips in scanning tunneling microscopes.

#### Talk 17: Wednesday 13:00-13:30

# Revealing attractive electron-electron interaction in a quantum dot by full counting statistics

Eric Kleinherbers<sup>1</sup>, Philipp Stegmann<sup>2</sup>, Jürgen König<sup>3</sup>

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Recent experiments [Nature **521**, 196 (2015) and Nat. Commun. **8**, 395 (2017)] have presented evidence for electron pairing in a quantum dot beyond the superconducting regime. Such an attraction between electrons can arise in a solid state environment due to coupling to bosonic modes (e.g. polarons, excitons or plasmons).

In my talk I will discuss that an attractive interaction, compared to a repulsive one, does generate pronounced correlations in electron transport. In particular, those correlations are revealed by a sign change of higher-order current correlators (generalized factorial cumulants) which can be obtained from the *full counting statistics* of electron transfer. Remarkably, those correlations are robust against a fast spin relaxation and, most importantly, are detectable even when typical experimental limitations of a charge detector are considered.

Publication:

E. Kleinherbers, P. Stegmann, and J. König 2018 New J. Phys. 20 073023

#### Talk 18: Wednesday 15:00-16:00

#### Structural Modifications and Quantum Interference to Tune Rectification in Molecular Junctions

#### Julio L. Palma

palmajl@psu.edu Department of Chemistry The Pennsylvania State University, Fayette, The Eberly Campus

Intrinsic molecular rectification is a desired feature in the design of future electronic devices at the nano and molecular scale. Previously, it has been shown that specific conformations and chemical modifications can be used to enhance molecular rectification of systems based on phenyl acetylene units, nonetheless, optimal values of rectification are usually present in higher energy conformers and not in minimum energy geometries. In this work, we study the role of quantum interference in molecular diodes and how this phenomenon can be used to enhance the rectification ratio. Our study consists on donor-bridge-acceptor (D-B-A) systems based on phenylene units and chemical modifications. Transport properties are calculated using the Green's functions technique and density functional theory (NEGF-DFT). Our results show that quantum interference together with chemical modifications could lead to high values of rectification in minimum energy conformers. These findings could lead to design principles of molecular devices and their application in fields where directional charge transport is desired.

#### Talk 19: Wednesday 16:30-16:45

#### Theoretical Studies on the Length Dependence of Molecular Rectification

#### Irvin Guzmán

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Molecular electronics is the branch that specializes on the study and development of different molecular systems and their arrangement to function as electronic components. One of the focus of molecular electronics is the design and study of devices that could transport charge in one direction but suppresses it in the opposite direction, this property is known as molecular rectification. On the present work, we characterized the dependence of intrinsic rectification ratio (RR) with respect the length of the system. The molecular junction was arranged in the usual Electrode-Molecule-Electrode set up, where the electrodes were gold nanowires attached to the molecules via thiolate anchoring groups. Our molecules are organized as Donor-Bridge-Acceptor (D-B-A), where the Donor and Acceptor regions are aromatic rings with amine and nitro substituents respectively and the bridge is based on acetylenes and phenylene units. We varied the number of bridge units and we found that there is a significant increase of the RR when the number of units is equal to 3. We found RR of up to 5.62 at 0.25 V and 3 phenylene units as a bridge. We aim to contribute in the future design of molecular electronics and the characterization of the rectification with respect the length to inspire possible synthesis of optimal molecular diodes.

#### Talk 20: Wednesday 16:45-17:00

#### Theoretical Studies of Coherent Transport in $\pi$ - $\pi$ Stacking Systems

Rafael Peña

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The study of different materials for the development of molecular electronics devices will provide with new advances in the fields of nanotechnology, photovoltaics and modern medicine. One of such materials are organic structures based on  $\pi$ - $\pi$  stacked systems. In this project we focus on the systematic study and characterization for different  $\pi$ - $\pi$  systems to understand the electron transport mechanism and the effects of structural modifications. The structures were connected to metallic gold electrodes in an electrode-molecule-electrode set up. We calculated molecular conductance values based on density functional theory and NEGF calculations. Anthracene, was used as the base molecule for this study, building structures of up to 4 layers. Systems with anthraquinone and hydroanthraquinone were also constructed to compare the differences in the conductance of the materials. Scaffolds were built to place the molecules in a more realistic environment and study their effect compared to the base models. We found that the conductance values vary slightly before and after the scaffold are used and that small chemical modifications could be used to design molecular switches based on  $\pi$ - $\pi$  systems.

#### Talk 21: Wednesday 17:30-18:30

#### **Coloquium at the Physics Institute**

#### Electron transport in stacked and gated 2D nano-structures: Lessons from calculations

Mads Brandbyge -- Technical University of Denmark (DTU)

Devices based on stacked van der Waals heterostructures of two-dimensional (2D) materials are promising candidates for future atomically thin, flexible electronics with properties that can be tuned by the electrostatic and dielectric environment.

In this talk I will present examples where we employ first principles transport calculations based on Density Functional Theory (DFT), which explicitly include the electrostatic gate potential and induced carriers. DFT is combined self-consistently with non-equilibrium Greens functions (NEGF) to study the effects of finite bias in devices [1,2]. I will discuss what we can learn from the DFT-NEGF calculations about f.ex. the role of the gate position in stacked devices [3], resistance of metallic edge-contacts to graphene [4], how an intrinsic, vertical dipole may be engineered and utilized in stacks involving the so-called Janustype di-chalcogenides, among other topics.

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#### Talk 22: Thursday 10:00-11:00

# Topological states and anomalous localization in non-Hermitian systems

Luis E. F. Foa Torres Universidad de Chile, Santiago, Chile

Recently, the search for topological states has reached non-Hermitian lattices (for a brief review see [1]), systems where non Hermiticity is used to model gains and losses (as in photonic crystals) or the effect of interactions (such as electron-electron and electron-phonon). Capital to this endeavor is the ability to build a proper bulk-boundary correspondence, a task that has gained much attention during the last year.

In this talk I will give an overview on recent results challenging the usual viewpoint in the theory of topological states that emerge when facing with non-Hermitian terms. One of such points being the occurrence of higher-order exceptional points where a macroscopic fraction of the states coalesce at a single point with a geometrical multiplicity of one [2]. At such points it may occur that the system becomes devoid of extended states (even for a pristine lattice), thereby challenging the idea that the boundary states may be connected to a bulk at all. Finally, I will comment on recent results providing a scheme to build such higher-order exceptional points in lattices [3, 4].

[1] V. M. Martinez Alvarez, J. E. Barrios Vargas, M. Berdakin, and L. E. F. Foa Torres, Eur. Phys. J. Spec. Top. (2018), <u>https://doi.org/10.1140/epjst/</u> <u>e2018-800091-5</u>

[2] V. M. Martinez Alvarez, J. E. Barrios Vargas, and L. E. F. Foa Torres, Phys. Rev. B 97, 121401(R) (2018).

[3] V. M. Martinez Alvarez, L. E. F. Foa Torres, to be published.

[4] Related references available at <a href="http://www.foatorres.com/publications/">http://www.foatorres.com/publications/</a>

#### Talk 23: Thursday 11:30-12:30

#### How General Relativity Helps to Design Valleytronic Nanodevices

Nikodem Szpak -- University of Duisburg-Essen

Graphene belongs to the fascinating class of Dirac materials where the quasiparticle excitations can be described by the Dirac equation. An additional valley degree of freedom can be used in a new type of valleytronic devices (in analogy to spintronics). Their main building block must be capable of manipulating the different valley polarizations. We proposed a strain based current splitter in which the effective gauge fields appearing in the system separate different valleys in space, similarly as the Stern-Gerlach experiment does to spins. To predict the current flow lines and design the system we studied the Dirac equation coupled to curvature and derived an analogue of geodesics. The semiclassical approach offers then an efficient ray tracing method, referred to as electron optics, which helps to better understand and optimize the device geometry. Thus obtained fully valley polarized currents can be measured and further processed by a precise placement of electronic contacts. We present the theory and the results of numerical simulations which prove the general concept.

#### Talk 24: Thursday 12:30-13:00

#### **Graphene transistors using TiO2**

Laura Serkovic -- Universidad Nacional Autónoma de México

In this work, we present a graphene field effect transistor GFET using a thin film of TiO2 as the dielectric layer. We show the different dopings obtained in different samples when using n-doped or p-doped silicon as a substrate and also how the doping in graphene changes due to its transfer process. This GFETs will be used for sensing molecules in the near future.

#### Talk 25: Thursday 13:00-13:30

#### Helium Nanodroplets at Ultra Cold Temperatures. The Problem of Excited States Calculation

A. Gamboa -- Universidad Autónoma del Estado de Morelos

<sup>4</sup>He presents a lot of unusual properties near absolute zero. Becoming a superfluid is perhaps the most known of these. Besides, it is possible to form very small nanodroplets, some of then of only a few tenths of atoms, surrounding a dopant molecule. They present a lot of interesting spectroscopic properties showing a very well defined peaks that are more commonly observed for systems in gas phase.

To be able to study of the dynamics of these systems is necessary to solve the Schrodinger's equation for many bodies. The complexity of the problem makes unfeasible the use of variational methods, making necessary to use a Diffusion Monte Carlo (DMC) approach.

DMC is exact for the calculation of the ground state of the system, but for the calculation of excited states is necessary a previous knowledge of the node of the wavefunction that one wants to calculate. Depending on the nature of the dopant molecule, sometimes is possible to make an estimation of these nodes making use of some suitable approximations. Nevertheless, when the potential between the molecule and the helium is very anisotropic, the correct estimation of the node becomes a difficult task.

In this work we present a Genetic Algorithm approach that has prove to be efficient for the exact calculation of the nodes of the excited states wavefunction making possible to study the dynamics of the nanodroplets even when the anisotropy of the potential is very big.

## Talk 26: Thursday 15:00-16:00

### Electron Transport in Molecular Junctions and Spin-dependent Chemistry

Vladimiro Mujica -- Arizona State University

#### Talk 27: Thursday 16:30-17:00

# Emulating Solid State Physics with Mechanical Waves: from Tunneling to Bloch Oscillations and Rainbow Trapping.

Rafael Méndez -- Universidad Nacional Autónoma de México

#### Talk 28: Thursday 17:00-17:30

## Macroscopic Coherence as an emergent property in molecular nanotubes

Giuseppe Luca Celardo -- Benemérita Universidad Autónoma de Puebla

Nanotubular molecular self-aggregates are characterized by a high degree of symmetry and they are fundamental systems for light-harvesting and energy transport. While coherent effects are thought to be at the basis of their high efficiency, the relationship between structure, coherence and functionality is still an open problem. We analyze natural nanotubes present in Green Sulfur Bacteria. We show that they have the ability to support macroscopic coherent states, i.e. delocalized excitonic states coherently spread over many molecules, even at room temperature. Specifically, assuming a canonical thermal state we find, in natural structures, a large thermal coherence length, of the order of 1000 molecules. By comparing natural structures with other mathematical models, we show that this macroscopic coherence cannot be explained either by the magnitude of the nearest-neighbour coupling between the molecules, which would induce a thermal coherence length of the order of 10 molecules, or by the presence of long-range interactions between the molecules. Indeed we prove that the existence of macroscopic coherent states is an emergent property of such structures due to the interplay between geometry and cooperativity (superradiance and super-transfer). In order to prove that, we give evidence that the lowest part of the spectrum of natural systems is determined by a cooperatively enhanced coupling (super-transfer) between the eigenstates of modular sub-units of the whole structure. Due to this enhanced coupling strength, the density of states is lowered close to the ground state, thus boosting the thermal coherence length. As a striking consequence of the lower density of states, an energy gap between the excitonic ground state and the first excited state emerges. Such energy gap increases with the length of the nanotube (instead of decreasing as one would expect), up to a critical system size which is close to the length of the natural complexes considered.

## Talk 34: Thursday 17:30-18:00

## **Microwave emulation experiments**

Thomas H. Seligman

## Talk 29: Friday 10:00-11:00

# Electronic transport through carbon chains and graphene p-n junctions

Jean-Christophe Charlier -- Université Catholique de Louvain

#### Talk 30: Friday 11:30-12:00

#### Laser-induced effects in graphite

José Eduardo Barrios Vargas<sup>1\*</sup>, Hernán L. Calvo<sup>2</sup>, Luis E. F. Foa Torres<sup>3</sup>

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The common classification of the electronic phases (insulator, semiconductor, semimetal and metal) of matter is based on spectral properties. However, the discovery of the topological insulators (TI) added a new kind of classification based on topological information carried by the eigenstates of the system. A topological insulator is a material that behaves as an insulator in the bulk and hosts conducting surface states, these surface states are like highways for electrons. The conducting surface states are weakly affected by disorder which is an attractive characteristic for applications. Even when thousands of known materials behave as topological insulators [1], these materials have challenges to incorporate in novel devices [2]. One research line aims at exploring new ways to induce topological electronic phases in common materials using laser illumination [3-6]. In this way the illuminated material may host a topological state, a phase commonly known as Floquet topological insulator [4]. In this work, we explore laser induced effects in graphite, where we find a bundle of conducting surface states.

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- [1] Zhang, T. et al. (2018), *arXiv*:1807.08756. Tang, F. et al. (2018), *arXiv*:1807.09744. Vergniory, M.G. et al. (2018), *arXiv*:1807.10271.
- [2] Lian, B. et al. PNAS 115 (43) 10938-10942 (2018).
- [3] Oka, T.; Aoki, H. Phys. Rev. B 79, 081406 (2009).
- [4] Lindner, N.H.; et al. Nat. Phys. 7, 490-495 (2011).
- [5] P. M. Perez-Piskunow et al. Phys. Rev. B 89, 121401(R) (2014).
- [6] H. L. Calvo et al. Phys. Rev. B 91, 241404 (2015).

#### Talk 31: Friday 12:00-12:30

#### Understanding the role of interfaces in 2D Magnetic Tunnel junctions

Simon M.-M. Dubois

#### Unité-Mixte de Physique CNRS-Thales, Palaiseau, France. Institute of Condensed Matter and Nanosciences, UCLouvain, Louvain-La-Neuve, Belgium.

Two-dimensional materials are promising candidates for use as tunnel barrier in atomically thin magnetic tunnel junctions (MTJs) [1]. High magneto resistance ratios have been predicted theoretically and recent progress in large scale manufacturing of these materials has paved the way to their integrations in functional devices. Yet, the experimental results available so far vary greatly depending on the integration pathways. Seeking for increased performances, it has been shown lately that direct CVD growth of tunnel barriers improves significantly the quality of the ferromagnet-2D materials interfaces [2-4]. Following these recent developments, new phenomena such as the bias induced reversal of the magneto resistance were reported [5]. Here, we show that first-principles calculations can provide direct insights into the close relation that links the interface morphology to its magneto resistive behaviour. In particular, we reports on the origin of TMR reversal in *h*-BN based MTJs with cobalt electrodes [5].

- 1 M. Piquemal-Banci et al., J. Phys. D. Appl. Phys. (2017), 50, 203002
- 2 S. Caneva *et al.*, Nano Lett. (2016), 16, 1250.
- 3 M.-B. Martin *et al.*, Appl. Phys. Lett. (2015), 107, 012408.
- 4 S. Caneva et al., ACS Appl. Mater. Interfaces (2017), 9, 29973.
- 5 M. Piquemal-Banci *et al.*, ACS Nano, (2018) to be published.

#### Talk 32: Friday 12:30-13:00

#### One way transport of charge and valley in graphene and topological states in metal-organic frameworks

Matias Berdakin

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We explore the generation of charge and valley polarized unidirectional transport in graphene bilayers [1]. With this aim we build on previous proposals [2,3] and show how one-way ambipolar charge and valley transport can be achieved in graphene bilayers under experimentally feasible conditions. Furthermore we analyze the valley polarization robustness among the presence of intervalley scattering in the system.

The second part of the talk would focus on the topological states in "*metal-organic frameworks*" and the chances of detecting them [4].

[1] M. Berdakin, J. E. Barrios Vargas, L. E. F. Foa Torres, to be published.

- [2] L. E. F. Foa Torres, V. Dal Lago, E. Suárez Morell, Phys. Rev. B. 93 [2016], 075438
- [3] V Dal Lago, E. Suárez Morell, L. E. F. Foa Torres, Phys. Rev. B. 96 [2017], 235409
- [4] M. Berdakin, L. E. F. Foa Torres, unpublished.

#### Talk 33: Friday 13:00-13:30

# Ab-initio tight binding models for transport and spectroscopies

Andrés Botello Méndez -- Universidad Nacional Autónoma de México

In this talk, I will describe the methodology used for extracting tight binding parameters from ab-initio DFT calculations using a projection of plane-waves into Wannier functions. The motivation behind this work is to provide accurate tight-binding models to be used in the computation of transport and spectroscopic properties of 2D materials. The presented methodology has been used to extract an accurate tight binding model for graphene under uniform strain.