

Conference on
Transport at the Nanoscale

25 - 29 September 2017

Centro Internacional de Ciencias A.C.
Cuernavaca, Mexico

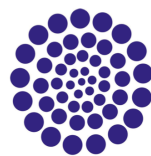
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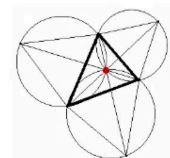


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24. Gerardo Naumis (Mexico)
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31. Isaac Rodríguez-Vargas (Mexico)
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37. Laura Serkovic-Loli (Mexico)
38. Thomas Stegmann (Mexico)
39. Thomas Seligman (Mexico)
40. Thijs Stuyver (Belgium)
41. Nikodem Szpak (Germany)
42. María Vozmediano (Spain)
43. Dietrich Wolf (Germany)

	Monday	Tuesday	Wednesday	Thursday	Friday
10:00 am	1) Nitzan	7) Heller	13) Vozmediano	17) Palma	23) Pastawski
10:30 am					
11:00 am	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:30 am					
12:00 am	2) Herrmann	8) Szpak	14) Wolf	18) Stuyver	24) Barrios-Vargas
12:30 am					
1:00 pm	3) Carrillo-Bastos	9) Castro-Villarreal	15) Sandler	19) Rojas-Iñiguez	25) Serkovic-Loli
1:30 pm					
2:00 pm	Lunch	Lunch	Lunch	Lunch	Lunch
2:30 pm					
3:00 pm	4) Rodriguez-Vargas	10) Barraza-Lopez	16) Foa-Torres	20) Ortiz	26) Mujica
3:30 pm					
4:00 pm	Coffee Break	Coffee Break	Poster session	Coffee Break	Coffee Break
4:30 pm	5) Lorke	11) Franco		21) Bustos-Marún	27) Celardo
5:00 pm	6) Stegmann	12) Naumis		22) Sadurní	28) Seligman
5:30 pm					
6:00 pm			Conference dinner at the Cave		
6:30 pm					
7:00 pm					
7:30 pm					
8:00 pm					

- 1) A. Nitzan: *Transport and optical response in illuminated molecular junctions*
- 2) C. Herrmann: *Pathways in molecular conductance and spin coupling*
- 3) R. Carrillo-Bastos: *Wave Packets Dynamics in deformed graphene*
- 4) I. Rodriguez-Vargas: *Self-similar transport in graphene-based complex structures*
- 5) A Lorke: *Carrier Dynamics in Self-Assembled Quantum Dots*
- 6) T. Stegmann: *Transport in graphene and disordered networks*
- 7) E. Heller: *Ultrafast and Raman spectroscopy for the masses of carbon atoms*
- 8) N. Szpak: *Precise electronic and valleytronic nanodevices based on strain engineering in graphene*
- 9) P. Castro-Villarreal: *Pseudomagnetic field in curved graphene*
- 10) S. Barraza-Lopez: *Beenakker's model for charge transport through graphene, and an overview of 2D materials with structural degeneracies*
- 11) I. Franco: *Atomistic modeling of electromechanical spectroscopies in molecular junctions*
- 12) G. Naumis: *Topological modes in time-periodically driven strained graphene nanoribbons*
- 13) M. Vozmediano: *Chiral anomaly and axial gauge fields in Weyl matter*
- 14) D. Wolf: *Statistical Modelling of Decoherence*
- 15) N. Sandler: *Unique features of transport in graphene revealed by mechanical deformations*
- 16) L. Foa-Torres: *From Floquet topological Insulators to Floquet isolators: A path from topological switching to transport steering*
- 17) J. Palma: *Molecular rectification enhancement and charge transport control based on conformational and chemical modifications*
- 18) T. Stuyver: *Exploring Electrical Currents through Nanographenes: Visualization and Tuning of the Through-Bond Transmission Paths.*
- 19) F. Rojas-Iñiguez: *Quantum Fisher Information and the spin- and charge-current conductivities in spin-orbit coupled systems*
- 20) Y. Ortiz: *Vibrational modes, transport and spontaneous symmetry breaking in carbon chains*
- 21) R. Bustos-Marún: *Geometric rectification for nanoscale vibrational energy harvesting*
- 22) E. Sadurní: *Hidden symmetry in dimeric complexes*
- 23) H. Pastawski: *Decoherent time-dependent transport beyond Landauer-Büttiker: a Quantum Drift alternative to Quantum Jumps*
- 24) J. Barrios-Vargas: *Charge transport in hydrogenated polycrystalline graphene*
- 25) L. Serkovic-Loli: *Chemical vapor deposition graphene grown on dielectric substrates through catalyst metal*
- 26) V. Mujica: *The Role of hydrogen bond in electron transport in molecular junctions*
- 27) G. Celeardo: *Cooperative effects and long range interaction: Cooperative shielding*
- 28) T. Seligman: *A fantasy about quasi 1D carbon molecules with decorations as quantum registers*

Talk 1: Monday 10:00-11:00

Transport and optical response in illuminated molecular junctions

Abraham Nitzan
University of Pennsylvania

The interaction of light with molecular conduction junction is attracting growing interest as a challenging experimental and theoretical problem on one hand, and because of its potential application as a characterization and control tool on the other. From both its scientific aspect and technological potential it stands at the interface of two important fields: molecular electronics and molecular plasmonics. I shall review the present state of the art of this field and our work on optical response, switching, Raman scattering, temperature measurements, light generation and photovoltaics in such systems.

Talk 2: Monday 11:30-12:30

Pathways in molecular conductance and spin coupling

Carmen Herrmann¹

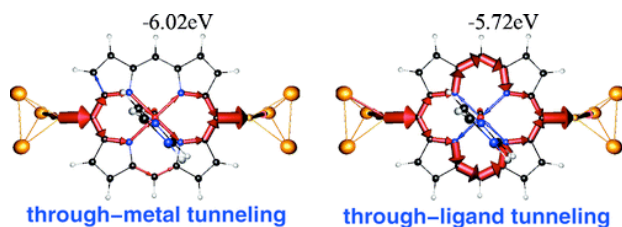
¹*Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, 20146 Erlangen, Germany*

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.



[1] T. Steenbock, J. Tasche, A. Lichtenstein, C. Herrmann, *J. Chem. Theory Comput.* **11**, 5651 (2015).

[2] T. Steenbock, C. Herrmann, submitted.

[3] G. C. Solomon, C. Herrmann, T. Hansen, V. Mujica, M. A. Ratner, *Nature Chem.* **2**, 223 (2010).

[4] R. Hayakawa, M. A. Karimi, J. Wolf, T. Huhn, M. S. Zöllner, C. Herrmann, E. Scheer, *Nano Lett.* **16**, 4960 (2016).

[5] C. Herrmann, G. C. Solomon, *J. Phys. Chem. C*, **114**, 20813 (2010).

[6] C. Herrmann, G. C. Solomon, M. A. Ratner, *J. Am. Chem. Soc.* **132**, 3682 (2010).

[7] C. Herrmann, G. C. Solomon, M. A. Ratner, *J. Chem. Phys.* **134**, 224306 (2011).

Talk 3: Monday 12:30-13:30

Wave Packets Dynamics in deformed graphene

Ramon Carrillo-Bastos¹ and Francisco Mireles²

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²Centro de Nanociencias y Nanotecnología de la UNAM, 22800 Ensenada, Baja California, México.

In monolayer graphene, out-of-plane strain-induced centro-symmetric deformations can be described as a six-folded pseudo-magnetic field in the low energy approximation [1]. It has been shown that such pseudo-magnetic field profiles can cause the formation of bound states [2], valley splitting, and valley filtering [3-5] of great interest in the realm of valleytronics and strain engineering. In this work, we study the dynamics of wave packets in graphene sheets that experiences local out-of-plane strain deformations in the form of Gaussian bumps. The study is carried out within the continuum Dirac Hamiltonian for graphene employing the time splitting spectral method for the time evolution operator. We present numerical results for different initial conditions (angle and energy of incidence) that shows wave packet focusing and beam splitting effects that can be exploited in the implementation of valleytronic devices. [1] Yang et al., J. Appl. Phys. 112, 073710; [2] Carrillo-Bastos et al. Phys. Rev. B 90, 041411R; [3] Settnes, et al., arXiv:1608.04569; [4] Milovanovic and Peeters, arXiv:1610.09916; [5] Carrillo-Bastos et al., Phys. Rev. B 94, 125422.

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Talk 4: Monday 15:00-16:00

Self-similar transport in graphene-based complex structures

I. Rodríguez-Vargas

Unidad Académica de Física, Universidad Autónoma de Zacatecas, Calzada Solidaridad Esquina
Con Paseo de la Bufa S/N, Zacatecas 98060, Zacatecas, México.

The two-dimensional nature of graphene offers an ideal platform to study electronic transport in complex geometries [1]. In principle, countless complex structures with unique geometrical characteristics can be achievable by nanopatterning and substrate engineering. The possible dynamics of electrons in these structures are intriguing for both the fundamental and technological standpoints.

In this talk, we address electron transport through a novel geometric structure in graphene [2]. The key ingredient of this structure is self-similarity. We propose a Cantor-like quantum potential achieved by engineering the substrate in which graphene is deposited. We found remarkable scaling (self-similarity) evidence in a measurable physical property, the linear-regime conductance. As we are dealing with charge carriers in graphene, it is natural to adopt a quantum relativistic description through the Dirac equation, hence the conductance correspond to this theoretical framework as well as to the guidelines of the Landauer-Büttiker formalism for charge transport. We also discuss the reasons to consider “self-similar transport” as a unique and exotic phenomenon in graphene.

1. E. van Veen, S. Yuan, M. I. Katsnelson, M. Polini and A. Tomadin, Quantum transport in Sierpinski carpets, *Phys. Rev. B* **93**, 115428 (2016).
2. H. García-Cervantes, L. M. Gaggero-Sager, D. S. Díaz-Guerrero, O. Sotolongo-Costa, I. Rodríguez-Vargas, Self-similar conductance patterns in graphene Cantor-like structures, *Scientific Reports* **7**, 617 (2017).

Talk 5: Monday 16:30-17:30

Carrier Dynamics in Self-Assembled Quantum Dots

Axel Lorke

Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Self-assembled InAs nano-islands are ideal model systems to study the energy structure of fully confined, interacting few-electron quantum systems [1]. Furthermore, when they are embedded in a suitable field-effect transistor structure and in tunneling contact with a two-dimensional electron system, it is possible to inject carriers into excited states and prepare non-equilibrium configurations [2]. This way, detailed information can be obtained on quantization as well as direct and exchange Coulomb interaction among the carriers. Furthermore, the dynamics of spin-forbidden transitions between electronic states can be studied by time-resolved transconductance spectroscopy [3]. While these methods offer time resolution down to the nanosecond scale, they are ensemble measurements and thus limited in their energy resolution. Optical spectroscopy, on the other hand, which is able to address a single quantum dot, enables energy resolution down to $\approx 1\mu\text{eV}$. Using time-resolved resonance fluorescence spectroscopy, [4] it is possible to study the dynamics of carriers, which interact among themselves as well as with a tunnel-coupled reservoir. This includes non-equilibrium processes such as Auger recombination [5] and capture of optically excited carriers [6] as well as near-equilibrium processes such as electron tunneling between the reservoir and the quantum dot. The latter process can be monitored with single electron, single shot resolution. The resulting optical random telegraph signal gives the full counting statistics of tunneling into and out of an interacting many-body charge carrier system.

- [1] P. M. Petroff, A. Lorke, and A. Imamoglu; *Physics Today* **54**, 46 (2001).
- [2] B. Marquardt, M. Geller, B. Baxevanis, D. Pfannkuche, A. D. Wieck, D. Reuter and A. Lorke; *Nature Commun.* **2**, 209 (2011)
- [3] K. Eltrudis, A. Al-Ashouri, A. Beckel, A. Ludwig, A. D. Wieck, M. Geller, and A. Lorke; *Appl. Phys. Lett.*, accepted (2017)
- [4] A. Kurzmann, B. Merkel, P. A. Labud, A. Ludwig, A. D. Wieck, A. Lorke, and M. Geller; *Phys. Rev. Lett.*, **117**, 017401 (2016).
- [5] A. Kurzmann, A. Ludwig, A. D. Wieck, A. Lorke, and M. Geller; *Nano Lett* **16**, 3367 (2016).
- [6] A. Kurzmann, A. Ludwig, A. D. Wieck, A. Lorke, and M. Geller; *Appl. Phys. Lett.* **108**, 263108 (2016).

Talk 6: Monday 17:30-18:30

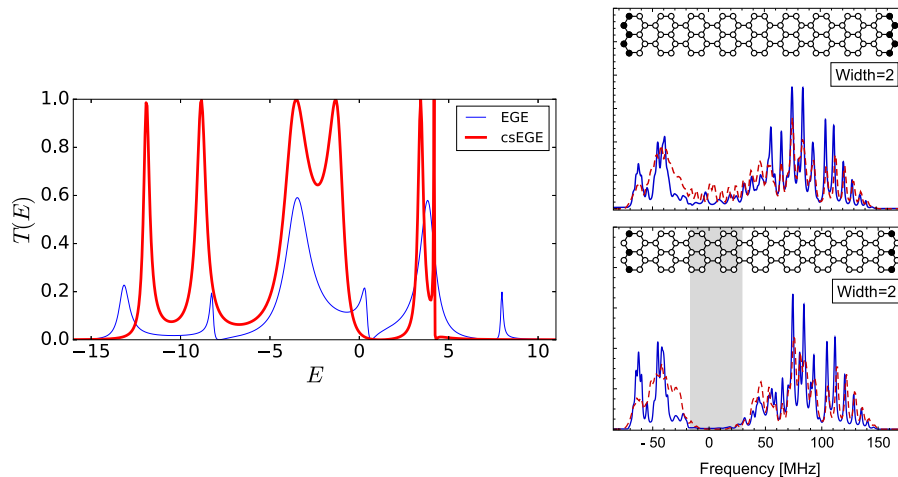
Transport in graphene and disordered networks

Thomas Stegmann

Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México. Cuernavaca, Mexico

In the first part of this talk, we will discuss the electron transport in small graphene nanoribbons by means of microwave emulation experiments and tight-binding calculations. In particular, it is investigated under which conditions a transport gap can be observed. Our experiments provide evidence that armchair ribbons of width $3m+2$ with integer m are metallic and otherwise semiconducting, whereas zigzag ribbons are metallic independent of their width. The contact geometry, defining to which atoms at the ribbon edges the source and drain leads are attached, has strong effects on the transport. If leads are attached only to the inner atoms of zigzag edges, broad transport gaps can be observed in all armchair ribbons as well as in rhomboid-shaped zigzag ribbons. [1]

In the second part of this talk, we will discuss the coherent transport of excitations in disordered interacting networks, which are modeled by embedded Gaussian random matrix ensembles (EGE). The transport is enhanced significantly whenever centrosymmetric embedded ensembles (csEGE) are considered. In this case the transmission shows numerous resonances of perfect transport. Analyzing the transmission by spectral decomposition, we find that centrosymmetry induces strong correlations and enhances the extrema of the distributions. This suppresses destructive interference effects in the system and thus causes backscattering-free transmission resonances that enhance the overall transport. [2]



[1] T. Stegmann, J.A. Franco-Villafañe, U. Kuhl, F. Mortessagne, T.H. Seligman, *Transport gap engineering by contact geometry in graphene nanoribbons: Experimental and theoretical studies on artificial materials*, Phys. Rev. B **95**:035413 (2017)

[2] A.Ortega, T. Stegmann, L. Benet, *Efficient quantum transport in disordered interacting many-body networks*, Phys. Rev. E **94**, 042102 (2016)

Talk 7: Tuesday 10:00-11:00

**Ultrafast and Raman Spectroscopy for the Masses of Carbon
atoms**

E. J. Heller

*Department of Physics and Department of Chemistry and Chemical Biology
Harvard University*

The spectroscopy of graphene, both ultrafast pulse-probe and slow (e.g. Raman) is undergoing a revolution in its paradigms, due ultimately to finally freeing up the electronic transition moment to depend on nuclear coordinates (so-called non-Condon effects), which has the effect of making indirect transitions more likely and instantaneous at the moment of absorption or emission. Agreement with experiment is greatly improved with a simpler set of assumptions.

Talk 8: Tuesday 11:30-12:30

Precise electronic and valleytronic nanodevices based on strain engineering in graphene

Nikodem Szpak¹, Thomas Stegmann²

¹University of Duisburg-Essen, Duisburg, Germany

²Universidad Nacional Autonoma de Mexico, Cuernavaca, Mexico

Abstract:

Graphene based nanodevices can be made so small that quantum transport phenomena play a crucial role in their functionality. We will present several such systems and discuss the theoretical and numerical models which are helpful in the understanding and efficient prediction of their electronic properties.

As examples, planar graphene with out-of-plane deformations and bent carbon nanotubes will be discussed as deformation/pressure nano-sensors and valley filters/polarizers. Precise combination of the curvature, magnetic and the pseudo-magnetic fields enables to control the quantum transport in these systems and gives rise to phenomena such as directing and focusing of currents depending on the deformation, placement of contacts and valley polarization. They can be applied in new types of graphene based electronic and valleytronic nanodevices.

Keywords: Graphene, Valleytronics, Quantum Transport, Strain, Effective Gauge Fields, Curved Space.

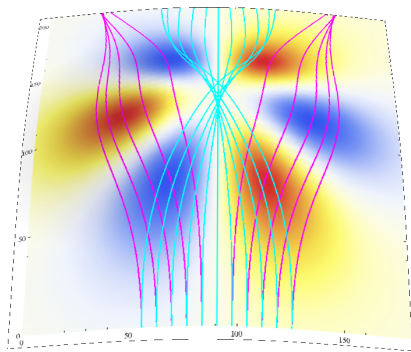


Figure 1: Theoretical model of current lensing and valley filtering based on classical trajectories

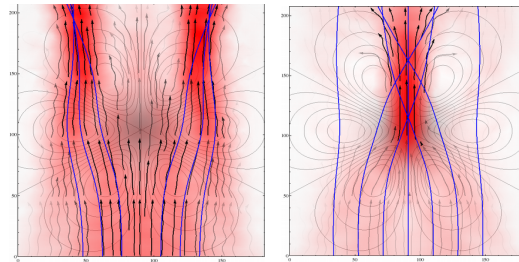


Figure 2: Numerical model of current lensing and valley filtering based on quantum transport calculations

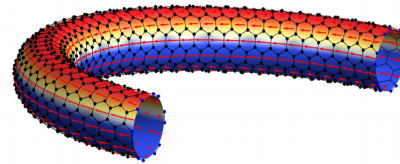


Figure 3: Artificial gauge fields due to strain in deformed carbon nanotubes also influence their current flow profiles and valley polarization

References:

1. T. Stegmann and N. Szpak, *New J. Phys.*, 18 (2016) 053016

Talk 9: Tuesday 12:30-13:30

Pseudomagnetic field in curved graphene

Pavel Castro Villarreal

PTC-Facultad de Ciencias en Física y Matemáticas

Universidad Autónoma de Chiapas

The general covariance of the Dirac equation is exploited in order to explore the curvature effects appearing in the electronic properties of graphene. Two physical situations are then considered: the weak curvature regime, with $|R| < 1/L^2$, and the strong curvature regime, with $1/L^2 \ll |R| < 1/d^2$, where R is the scalar curvature, L is a typical size of a sample of graphene, and d is a typical size of a local domain where the curvature is pronounced. In the first scenario, we found that the curvature transforms the conical nature of the dispersion relation due to a shift in the momentum space of the Dirac cone. In the second scenario, the curvature in the local domain affects the charge carriers in such a manner that bound states emerge; these states are declared to be pseudo-Landau states because of the analogy with the well known Landau problem; here the curvature emulates the role of the magnetic field. Seeking more tangible curvature effects we calculate, e.g., the electronic internal energy of graphene in the small curvature regime and give an expression for the ground state energy in the strong curvature regime.

Talk 10: Tuesday 15:00-16:00

Beenakker's model for charge transport through graphene, and an overview of 2D materials with structural degeneracies

Salvador Barraza-Lopez

Associate Professor. Department of Physics. University of Arkansas

sbarraza@uark.edu

An attempt will be made in this presentation to discuss two dissimilar topics that are unified by the main title of this workshop: (a) charge transport and (b) novel two-dimensional materials. On the topic of transport, I will describe a model put forth by the Leiden team in 2007 [1-4] to discuss charge transport through short graphene-metal junctions (that somehow competed with the diffusive model introduced by das Sarma and coworkers, which will not be discussed here). The basic result is that a full quantum treatment of the problem yields a Dorokhov [5] distribution of electrons that is not-normal (non-gaussian to be more precise), but it rather peaks at zero probability and unity probability, as if these electrons were classical particles, despite of the full quantum treatment. (Pierre Melo contributed to these ideas too [6]). Limitations of the model will also be discussed. I will use the remainder of time to introduce to the audience basic physical consequences of reduced structural symmetries on 2D materials beyond graphene. The message from this second part is that structural reduced symmetries are prominent in 2D materials, and these reduced symmetries lead to two-dimensional structural (i.e., non-topological) phase transitions [7-10].

References:

- [1] J. Tworzydło, B. Trauzettel, M. Titov, A. Rycerz, and C. W. J. Beenakker. *PRL* **96**, 246802 (2006)
- [2] C. W. J. Beenakker *Rev. Mod. Phys.* **80**, 1337 (2008)
- [3] S. Barraza-Lopez, M. Vanevic, M. Kindermann, and M.-Y. Chou. *PRL* **104**, 076807 (2010)
- [4] S. Barraza-Lopez, M. Kindermann, and M.-Y. Chou. *Nano Lett.* **12**, 3424 (2012)
- [5] O.N. Dorokhov. *Solid State Commun.* **51**, 381 (1984)
- [6] P.A. Mello, P. Pereyra, and N. Kumar, *Ann. Phys. (N.Y.)* **181**, 290 (1988)
- [7] M. Mehboudi, A.M. Dorio, W. Zhu, A. van der Zande, H.O.H. Churchill, A.A. Pacheco-Sanjuan, E.O. Harriss, P. Kumar, and S. Barraza-Lopez. *Nano Lett.* **16**, 1704 (2016)
- [8] M. Mehboudi, B. M. Fregoso, Y. Yang, W. Zhu, A. van der Zande, J. Ferrer, L. Bellaiche, P. Kumar, and S. Barraza-Lopez. *PRL* **117**, 246802 (2016)
- [9] A review of the electronic and optical properties of strained graphene and other similar 2D materials. G. G. Naumis, S. Barraza-Lopez, M. Oliva-Leyva, and H. Terrones. *Rep. Prog. Phys.* (in press, 2017).
- [10] K. Chang, et al. *Science* **353** 274 (2016)

Talk 11: Tuesday 16:30-17:30

Atomistic modeling of electromechanical spectroscopies in molecular junctions

Ignacio Franco
Rochester University

We present theoretical and computational advances toward the atomistic modelling of experiments that simultaneously measure the electric and mechanical properties of single-molecules in the context of nanoscale junctions. At the methodological level, we: (i) Establish well-defined conditions in which the Landauer steady-state approximation can be used to capture time-dependent currents through thermally fluctuating junctions. These criteria can be employed to develop effective modeling strategies for transport through molecular junctions in interaction with a fluctuating environment, as is necessary to describe experiments. (ii) Introduce an accurate and computationally efficient strategy to capture non-reactive metal-molecule interactions that adapts the Tkatchenko-Scheffler scheme for van der Waals interactions into a simple and transferable classical force field. The strategy allows for classical molecular dynamics simulation with the accuracy of high-level electronic structure methods but for system sizes and timescales that go well beyond what can be achieved with first principle methods. Such methods are then employed to: (i) Quantitatively simulate and atomistically understand experiments that measure the conductance of a single polyfluorene on Au(111) as a continuous function of its length, and; (ii) Explore the ability of force-conductance measurements to inform, at the single-molecule limit, about molecular recognition events through hydrogen bonds.

Talk 12: Tuesday 17:30-18:30

Topological modes in time-periodically driven strained graphene nanoribbons

Gerardo G. Naumis, Pedro Román-Taboada
Instituto de Física, UNAM

In this talk we will study the emergence of electronic non-trivial topological flat bands in time-periodically driven strained graphene. As a model, we use a tight binding approach based on the Floquet formalism. In particular, we will focus on uniaxial spatially periodic strain since we show that it can be mapped onto an effective one-dimensional system, leading in the static case to a fractal spectrum akin to the Hofstadter butterfly with several localization transitions and Van Hove singularities. Then, two kinds of time-periodic driving are considered: a short pulse (delta kicking) and a sinusoidal variation (harmonic driving). Even though the study case is gapless, we find that topologically non-trivial flat bands emerge not only at zero-quasienergy but also at the limits of the Floquet zone. Both kinds of flat bands are thus understood as dispersionless bands joining two inequivalent touching band points with opposite Berry phase. This is confirmed by explicit evaluation of the Berry phase in the touching band points' neighborhood. Using that information, the topological phase diagram of the system is built. This phase diagram and the topological modes are in excellent agreement with numerical calculations. Finally, we will discuss results concerning the Dirac equation for studying time-driving strain. This leads to a dressing of the Dirac cones with Arnold tongues, since the system is described by an effective Mathieu equation, i.e., by a simple parametric pendulum.

Talk 13: Wednesday 10:00-11:00

Chiral anomaly and axial gauge fields in Weyl matter

Maria A. H. Vozmediano

Instituto de Ciencia de Materiales de Madrid and CSIC

After the synthesis of graphene (massless Dirac fermions in 2+1 dimensions) in 2005 a whole new branch of topological materials has emerged which constitute novel physical realizations of high energy systems. Weyl semimetals (WSM) (the 3D graphene) are a material realization of Lorentz violating massless QED in (3+1) dimensions. The recent experimental confirmation has opened a new lab to explore anomaly related phenomena, and a number of experimental observations have already been reported. In graphene, lattice deformations couple to the electronic current in the form of "elastic gauge fields" axial in nature. In this talk we will see that elastic axial gauge fields are also present in the Weyl semimetals. Among the new response functions associated to them, we will show that WSM have an intrinsic Hall viscosity whose coefficient is related to the AAA triangle anomaly. A novel strain-induced chiral magnetic effect will also be present.

References

- “Elastic gauge fields in Weyl semimetals”, A. Cortijo, Y. Ferreira, K. Landsteiner, and M. A. H. Vozmediano, *Phys. Rev. Lett.* 115, 177202 (2015).
- “Visco elasticity in 2D materials”, A. Cortijo, Y. Ferreira, K. Landsteiner, and M. A. H. Vozmediano, *2D Materials* 3, 011002 (2016)
- “Strain induced Chiral Magnetic Effect in Weyl semimetals”, A. Cortijo, D. Kharzeev, K. Landsteiner, and M. A. H. Vozmediano, *Phys. Rev. B* 94, 241405(R) (2016).

Talk 14: Wednesday 11:30-12:30

Statistical Modelling of Decoherence

Dietrich E. Wolf

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Since Pauli's derivation of a quantum master equation (1928) the relation between decoherence of single (quasi-) particle states and irreversibility has been known. Decoherence is the reason for Ohmic resistance in electronic transport. Recently we proposed that the events, which lead to decoherence, are localized at randomly chosen sites. Their average distance is the decoherence length. This leads to a significant reduction of the computational effort for the calculation of transport phenomena, in particular for weak decoherence, or in one dimension. As an example, the conductance of DNA segments was calculated for different nucleotid sequences and compared with experiments [1]. The probability distribution of the decoherence sites has experimentally accessible consequences: A Poisson distribution leads to a metal-insulator transition at a threshold disorder in a one-dimensional Anderson model, while strong localization is suppressed by a more uniform spatial distribution of decoherence sites [2]. The model has lately been extended to include inelastic scattering inside the system between the source and the drain. This gives new insight, how the single particle distribution function deviates from the Fermi-Dirac equilibrium distribution [3].

[1] Matias Zilly, Orsolya Ujsághy, Dietrich. E. Wolf, *Conductance of DNA molecules: Effects of decoherence and bonding*, Phys. Rev. B **82**, 125125 (2010)

[2] Thomas Stegmann, Orsolya Ujsághy, Dietrich. E. Wolf, *Localization under the effect of randomly distributed decoherence*, Eur. Phys. J. B **87**, 30 (2014)

[3] Thomas Stegmann, Orsolya Ujsághy, Dietrich. E. Wolf, *Quantum transport under the effect of decoherence, energy relaxation and dissipation*, preprint (2017)

Talk 15: Wednesday 12:30-13:30

Unique features of transport in graphene revealed by mechanical deformations

N. Sandler

Ohio University

The coupling of geometrical and electronic properties is a promising venue to engineer properties in graphene and other two-dimensional materials. In fact, different regimes are achieved by a proper manipulation of confinement and strain fields, as shown in recent experiments on nanobubbles, drumheads oscillating membranes, and narrow strips deposited on patterned SiC substrates [1] among others. Not surprisingly, mechanical deformations can also be used to uncover unique properties of electronic transport in regimes where electron interactions may play an irrelevant or a dominant role. In recent work, we have explored specific geometries that exploit the mechanical flexibility of graphene membranes in these two different regimes. In the first case, we analyzed properties of linearly-shaped strained regions that form naturally or in a controlled manner when graphene is deposited on appropriate substrates. Electronic transport in this case is well describe by non-interacting electrons under the effect of a pseudo-magnetic field used to represent the deformation [2]. In the second case, we use a symmetric out-of-plane deformation to investigate the elusive Kondo regime in graphene, expected to appear when a magnetic impurity is deposited on top of the material. By using strain, we demonstrate the existence of a peculiar Kondo regime and suggest experimental settings where it can be detected.

[1] N. Levy, et al. Science 329, 544 (2010). T. Mashoff, et al. Nano Lett. 10, 461 (2010). N. Klimov, et al. Science 336, 1557 (2012). Baringhaus, et al. Nature 506, 349 (2014). [2] R. Carrillo-Bastos et al., Phys. Rev. B 94, 125422 (2016). Y. Wu, et al to appear in Nano Letters.

Talk 16: Wednesday 15:00-16:00

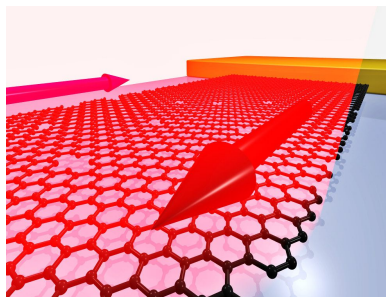
From Floquet topological Insulators to Floquet isolators: A path from topological switching to transport steering

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Light-matter interaction is at the heart of intriguing phenomena and has led to many practical applications, many of them in characterization. But beyond characterization, several studies have gone deeper into actually using light to modify the electrical properties of a material. This can be done, for example, by using light to switch off the conduction in graphene [1,2] (or other materials [3]), thereby allowing to tune the material's response with optical means, or even inducing tunable topological states in materials that would otherwise lack them [1,2,4,5,6,7,8] (i.e. a *Floquet topological insulator* [4]). The latter would expand the playground of topological insulators to a broader set of materials. The recent experimental realization of laser-induced bandgaps at the surface of a topological insulator [3] has added much interest to this area.



In this talk I provide an overview of our recent works in this field with a focus on the generation of Floquet chiral edge states in graphene [6,9,10], and other materials including topological insulators [8,11], and their Hall response [12]. We also show how light-matter interaction could be used to realize a *Floquet isolator* [13, 14], a system where transmission can occur only between say lead L and lead R but not in the opposite direction. This opens a door to a type of one-way transport that has been missing from the toolkit of available electronic devices.

- [1] T. Oka and H. Aoki, Phys. Rev. B **79**, 081406 (2009).
- [2] H. L. Calvo, H. M. Pastawski, S. Roche, and L. E. F. Foa Torres, Appl. Phys. Lett. **98**, 232103 (2011); H. L. Calvo, P. M. Perez-Piskunow, S. Roche, and L. E. F. Foa Torres, Appl. Phys. Lett. **101**, 253506 (2012).
- [3] Y. H. Wang, H. Steinberg, P. Jarillo-Herrero, and N. Gedik, Science **342**, 453 (2013).
- [4] N. H. Lindner, G. Refael, and V. Galitski, Nat. Phys. **7**, 490 (2011).
- [5] T. Kitagawa, T. Oka, A. Brataas, L. Fu, and E. Demler, Phys. Rev. B **84**, 235108 (2011).
- [6] P. M. Perez-Piskunow, G. Usaj, C. A. Balseiro, and L. E. F. Foa Torres, Phys. Rev. B **89**, 121401(R) (2014).
- [7] E. Suárez Morell and L. E. F. Foa Torres Phys. Rev. B **86**, 125449 (2012).
- [8] H. L. Calvo, L. E. F. Foa Torres, P. M. Perez-Piskunow, C. A. Balseiro and G. Usaj, Phys. Rev. B **91**, 241404(R) (2015).
- [9] G. Usaj, P. M. Perez-Piskunow, L. E. F. Foa Torres, and C. A. Balseiro Phys. Rev. B **90**, 115423 (2014); P. M. Perez-Piskunow, L. E. F. Foa Torres and G. Usaj, Phys. Rev. A **91**, 043625 (2015).
- [10] D. A. Lovey, G. Usaj, L. E. F. Foa Torres, C. A. Balseiro, Phys. Rev. B **93**, 245434 (2016).
- [11] V. Dal Lago, M. Atala and L. E. F. Foa Torres, Phys. Rev. A **92**, 023624 (2015).
- [12] L. E. F. Foa Torres, P. M. Perez-Piskunow, C. A. Balseiro, and G. Usaj, Phys. Rev. Lett. **113**, 266801 (2014).
- [13] V. Dal Lago, E. Suárez Morell and L. E. F. Foa Torres, [arxiv:1708.03304](https://arxiv.org/abs/1708.03304).
- [14] Related publications available at <http://www.foatorres.com/publications/>

The image shows an artist view of Floquet topological states generated by laser illumination in graphene.

Talk 17: Thursday 10:00-11:00

Molecular rectification enhancement and charge transport control based on conformational and chemical modifications

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Abstract

The understanding of the electron transport mechanism in molecular systems, from single organic molecules to DNA sequences, is crucial if they are to be used as electronic devices. By now, it is well accepted that at short distances the charge transport occurs via coherent tunneling while at longer distances it occurs via incoherent hopping. Even though many questions remain unanswered about the details of each mechanism, we can start exploring molecular features that could lead us to a better design of devices and specific electronic functions.

In our research, we have studied the characterization of conformational and chemical modifications and their effect in electron transport. More specifically, we have focused in the enhancement of molecular rectification that could lead to a more efficient design of molecular diodes and electron injectors in photovoltaic systems.

A few words we will reserve at the end to present our attempts to characterize molecular modifications in DNA sequences to control the charge transport in the hopping regime.

Talk 18: Thursday 11:30-12:30

Exploring Electrical Currents through Nanographenes: Visualization and Tuning of the Through-Bond Transmission Paths.

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In this work, electrical currents through nanographenes, also known as polycyclic aromatic hydrocarbons, in molecular junctions under small bias are explored. More in detail, we focus on different configurations of contacts on benzene, anthracene, pentacene, phenanthrene, pyrene and coronene. We use previously established rules of thumb to rationalize the transport properties of the different systems studied.^{1,2} Furthermore, we visualize the local transmission³ through the systems with the help of the ARTAIOS code⁴ and demonstrate that the π -current prefers the direction of the shortest bond (i.e. the bond with the highest double bond character) upon entering the molecule from the contacts. As such, the idea of electrons propagating through double bonds from contact to contact, originating from one of the previously established selection rules for transmission based on curly arrow drawings,¹ seems to be more deeply rooted in the actual physical process of electron transport than previously anticipated. On the other hand, the σ -current behaves completely differently. This type of current generally prefers the shortest path from contact to contact, irrespective of the length of the bonds constituting this path. Finally, it is demonstrated that keto-groups (and cross-conjugating groups in general) can be used to seal off parts of the molecule for the current. No current flows through the sealed off part of the molecule under small bias and it does not influence the transmission spectrum of the considered system.⁵

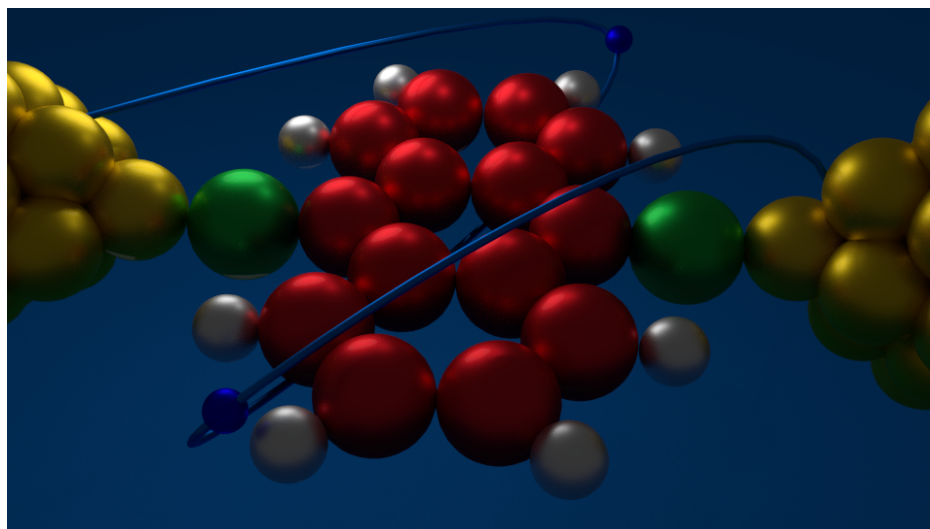


Fig. 1. Artist impression of an anthracene molecule incorporated in a molecular junction.

1. T. Stuyver, S. Fias, F. De Proft, P. Geerlings, *J. Phys. Chem. C* **119**, 26390 (2015).
2. T. Stuyver, S. Fias, F. De Proft, P. Geerlings, Y. Tsuji, R. Hoffmann *J. Chem. Phys.* **146**, 092310 (2017).
3. G. C. Solomon, C. Herrmann, T. Hansen, V. Mujica, M. A. Ratner, *Nat. Chem.* **2**, 223 (2010).
4. C. Hermann, L. Gross, T. Steenbock, G. C. Solomon, "Artaios – a code for postprocessing quantum chemical electronic structure calculations" (2010-2014).
5. T. Stuyver, N. Blotwijk, S. Fias, F. De Proft, P. Geerlings, *Chem. Eur. J.* (submitted).

Talk 19: Thursday 12:30-13:30

Quantum Fisher Information and the spin- and charge-current conductivities in spin-orbit coupled systems

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Quantum correlations are a central feature in Quantum Information and Quantum Computation. In particular, the Quantum Fisher Information (QFI) is known to be a good indicator of quantum entanglement in multipartite systems[1].

We investigate a relationship between an optimized form of QFI, over measurements in the spin subsystem, and the spin-spin susceptibilities in the linear response regime in spin-orbit coupled systems. This relation can be written in terms of the spin- and charge-optical conductive tensors through the known relations between these quantities and the spin-spin response function[2].

This result allows us to obtain a quantification of the hybrid spin-orbit correlations (entanglement, quantum discord) with Fisher information through the measurable observables associated to the spin or charge degree of freedom.

The authors would like to thank DGAPA and project PAPIIT IN105717 for financial support.

[1] Philipp Hauke et al Nature Physics 12,778 (2016)

[2] P. E. Iglesias y J. A. Maytorena Phys. Rev, B 82, 205324 (2010)

Talk 20: Thursday 15:00-16:00

**Vibrational modes, transport and spontaneous symmetry
breaking in carbon chains**

Yenni P. Ortiz

Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México. Cuernavaca, Mexico

Talk 21: Thursday 16:30-17:30

Geometric rectification for nanoscale vibrational energy harvesting

Raúl A. Bustos-Marín
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Universidad Nacional de Córdoba*

In recent years there has been an increasing interest in energy conversion of vibrational excitations. However, most of the proposed devices present problems for scaling them down to nanometric dimensions due to the very low output voltage and the wide vibrational spectrum of the environment. In this talk, we show how to realize a nanoscale vibrational energy harvester that operates on quantum mechanical principles. Our premise is that adiabatic quantum pumping can be used quite generally to convert random mechanical excitations into useful electrical work, which can have several advantages. The most important is that it avoids the use of classical rectification mechanisms as it is based on what we called geometric rectification. We show that this geometric rectification occurs naturally whenever impulsive initial conditions are applied to damped harmonic systems coupled to electronic reservoirs. We analyze an analytically solvable example consisting of a wire suspended over permanent charges where we find the condition for maximizing the charge pumped. We also studied the effects of coupling the system to a capacitor including the effect of back action forces and analyze the steady state voltage of operation. Finally, we show how quantum effects can be used to boost the performance of the proposed devices.

Talk 22: Thursday 17:30-18:30

Hidden symmetry in dimeric complexes

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A minimal array of single-orbital atomic sites is proposed with the property of having accidental level crossings when irregular (non-symmetric) configurations are reached. The broken dihedral symmetry of the resulting polymeric array implies that a hidden group operating in finite phase space is responsible for the effect. The corresponding Wigner functions are provided and analyzed.

Talk 23: Friday 10:00-11:00

Decoherent time-dependent transport beyond Landauer-Büttiker: a Quantum Drift alternative to Quantum Jumps

Horacio Pastawski and Lucas Fernández-Alcázar

Instituto de Física Enrique Gaviola y Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba

We developed a model for including decoherent processes in the quantum dynamics underlying time-dependent transport [1]. It is a dynamical formulation that boils down into a form of wave function whose local phase undergoes stochastic jump. Thus, decoherence arises from a random perturbation of the environment in a local basis. This is, by construction, more efficient than density matrix approaches. Using numerical calculations, we prove the equivalence among our dynamical model and the decoherent steady state transport through the resonant state $|0\rangle$ of a quantum dot that undergoes decoherence through contact with a voltage probe. We also reobtain the same results of steady state transport of the general cases described by the D'Amato-Pastawski model where decoherence occurs at any point of an extended sample [2]. Actual benefit of this model appears when one deal with time dependent decoherent transport. In this case, it provides great computational benefit over the Keldysh non-equilibrium Green's functions formalism, even when these are linearized in the form Generalized Landauer-Büttiker Equations [3]. We also apply this model to a two level system (TLS) that oscillates among $|0\rangle = |\uparrow\downarrow\rangle$ and $|1\rangle = |\downarrow\uparrow\rangle$. We show that our model recovers not only the exponential damping of the oscillations in the low perturbation regime, but also the bifurcation of the decoherence rates at a critical perturbation. Thus, our Quantum Drift model is able to show the quantum dynamical phase transition produced by the interaction with the environment. We perform the Loschmidt echo (LE) calculations to evaluate the decoherence in the TLS. We find that the pure states $|0\rangle = |\uparrow\downarrow\rangle$ and $|1\rangle = |\downarrow\uparrow\rangle$ are quite robust against the local perturbation. In contrast, the LE decays faster when the system is in a superposition state $\{|0\rangle + |1\rangle\}/\sqrt{2}$ or $\{|0\rangle - |1\rangle\}/\sqrt{2}$. These results are in agreement with the general trend recently observed in spin systems through NMR. that oscillates among $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$. We show that our model recovers not only the exponential damping of the oscillations in the low perturbation regime, but also the bifurcation of the decoherence rates at a critical perturbation. Thus, our Quantum Drift model is able to show the quantum dynamical phase transition produced by the interaction with the environment. We perform the Loschmidt echo (LE) calculations to evaluate the decoherence in the TLS. We against the local perturbation. In contrast, the LE decays faster when the system is in a superposition state $\{|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle\}/\sqrt{2}$. These results are in agreement with the general trend recently observed in spin systems through NMR. By considering a the dynamics in a many spins systems, we discuss how the Quantum Drift, applies to more general many-body cases. Complement with a Quantum Parallelism [4] strategy it out-runs the standard density matrix formalism. Finally, we show how the same strategy applies to non-local interactions that partially conserve momentum, a case more relevant for electronic transport.

[1] L.J. Fernández-Alcázar and H.M. Pastawski, *Decoherent time-dependent transport beyond the Landauer-Büttiker formulation: A quantum-drift alternative to quantum jumps*, Phys. Rev. A **91**, 022117 (2015)

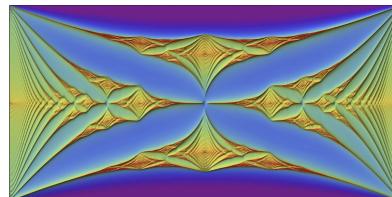
[2] C.J. Cattaena et al, *Generalized multi-terminal decoherent transport: recursive algorithms and applications to SASER and giant magnetoresistance* J. Phys.: Condens. Matter **26** (2014) 345304

[3] H.M. Pastawski *Classical and Quantum Transport from Generalized Landauer-Büttiker Equations II: Time dependent tunneling*. Phys. Rev. B **46** 4053 (1992)

[4] G.A. Álvarez et al, *Quantum Parallelism as a Tool for Ensemble Spin Dynamics Calculations* Phys. Rev. Lett. **101**, 120503 (2008)

Talk 24: Friday 11:30-12:30

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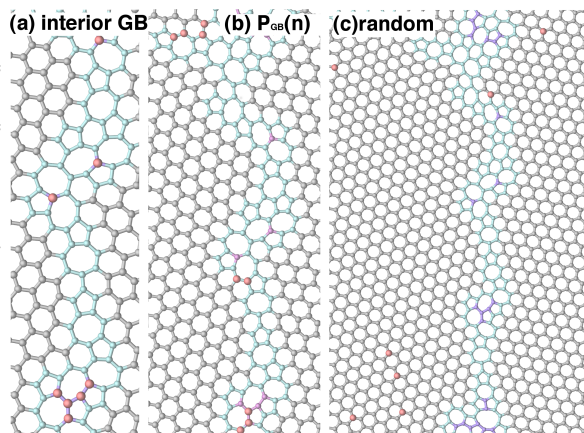
Charge transport in hydrogenated polycrystalline graphene

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Abstract

Two dimensional materials, like graphene, open the gate to a flexible nano-electronics. This nano-electronics requires affordable high-quality raw materials. Nowadays, the best relatively high quality mass production technique is chemical vapor deposition, which is mediated by nucleation and growth mechanisms. These processes produce a polycrystalline material which contains grain boundaries, dangling bonds and point defects; these defects give new electronic, magnetic and optical properties that can be useful in technology. Modeling these polycrystalline materials is quite challenging because the experimental samples usually have sizes of at least $1\mu\text{m}^2$ ($\sim 1 \times 10^9$ atoms). The real space formulation of the Kubo-Greenwood formula provides an efficient scheme for the evaluating spectral and transport properties. Using this formulation, we evaluate the charge transport properties of hydrogenated polycrystalline graphene. We find a strong correlation between the spatial distribution of the hydrogen and the transport properties. Charge transport is weakly sensitive to hydrogenation when adsorbates are confined to the grain boundaries, while a uniform distribution of hydrogen degrades the electronic mobility. This difference stems from the formation of the hydrogen-induced resonant impurity states, which are inhibited when the honeycomb symmetry is locally broken by the grain boundaries. Theoretically, there are many other adsorbates besides hydrogen that can give rise to resonant states, including PMMA, which is typically used to transfer graphene to a substrate.

Figure. Structural configuration of hydrogen adsorption in polycrystalline graphene. Panels show the case of polycrystalline graphene, with adsorption (a) on the interior grain boundary (GB) sites, (b) on the GB sites with a $P(n)$ distribution obtained by Monte Carlo simulations, and (d) randomly distributed throughout the sample (Adapted from Barrios Vargas et al. *2D Mater.* 4 (2017) 025009).



Talk 25: Friday 12:30-13:30

CHEMICAL VAPOUR DEPOSITION GRAPHENE GROWN ON DIELECTRIC SUBSTRATES THROUGH CATALYST METAL

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Graphene is a one-atom layer carbon material which has promising applications in electronics due to its high electron mobility and very low thickness. Many attempts have been made to clean the polymer residues after CVD graphene has been transferred to a substrate different from the one on which it was grown. However, this is not an easy task because a very thin layer of polymer remains on graphene, diminishing its electron mobility.

In this work, we managed to grow graphene on a thin copper film grown on a SiO₂/Si wafer [1]. Carbon atoms from methane diffuse through the copper film and produce graphene on the copper-SiO₂ interface. After etching the copper film, we obtain directly graphene on the SiO₂ surface, ready to measure its electronic conductivity parameters without the polymer contamination.

Our current goal is to refine this technique in order to directly grow graphene on copper patterns drawn on a SiO₂/Si wafer, thus avoiding the transference processes and the negative effects it has on the graphene film. This result could be of great use in the creation of microcircuits with graphene components.

This work was supported by PIIF 2016 IFUNAM and PAPIIT IA102217. We acknowledge technical support from Rodrigo Alejandro Gutiérrez Arenas and Cristina Zorrilla. We also acknowledge support from Graphenemex S.A. de C.V.

Keywords: Graphene, Chemical vapour deposition, Dielectric substrate

References:

[1] Ching-Yuan-Su et al., Nano Letters 11 (2011) 3612.

Talk 26: Friday 15:00-16:00

The Role of Hydrogen Bond in Electron Transport in Molecular Junctions

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The mapping into chemical bonds of transport channels in molecular junctions is a complex matter because of the non-Hermitian nature of the transmission operator. The use of local probe, e.g. STM, can shed new light on the properties of chemical bonds and how we can interpret in simple chemical terms the contribution to conductance of different bonds. While electron transport through covalent bonds has been extensively studied, in recent work the focus has been shifted towards hydrogen-bonded systems due to their ubiquitous presence in biological systems and their potential in forming nano-junctions between molecular electronic devices and biological systems.

We present here a theoretical and computational study of electron transport in molecular junctions involving hydrogen bonds in the quasi-resonant regime. This analysis allows us to interpret some key experimental results indicating that the inclusion of hydrogen bonding in a molecular junction significantly impacts its transport properties, a fact that has important implications for our understanding of transport through DNA, and nano-biological interfaces in general. In particular, we have explored the implications of quasiresonant transport in short chains of weakly-bonded molecular junctions involving hydrogen bonds to interpret recent experiments by Nishino *et al* and where, contrary to conventional chemical intuition, conduction through H-bonded chains was found to be larger than that through alkane chains, with a turnover region at a threshold length of about 13Å. We explain this experimental finding as the effect of a Fano resonances close to the Fermi energy of the junction.

Talk 27: Friday 16:30-17:30

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Talk : **TITLE: Cooperative effects and long range interaction: Cooperative Shielding.**

ABSTRACT:

Cooperative effects in long range interacting systems are at the center of interest in many systems in physics such as cold atomic clouds, light harvesting systems, and trapped ions. Cooperative effects are at the heart of Superradiance and Supertransfer showing enhance energy transport efficiency and a robustness to noise. In the first part of the talk we will review the role of cooperativity in different physical systems, focusing on the role of long range interaction in determining cooperative behaviours. The second part of the talk will be devoted to discuss the interplay of cooperativity and noise in systems with long range interaction (many body spin systems and tight binding models). The main focus will be on Cooperative Shielding. Contrary to the common expectation that long-range interaction should necessarily induce an instantaneous spread of information in the thermodynamic limit, we show that, as the system size increases, the dynamics can actually become more confined into invariant subspaces. In such subspaces, the dynamics is effectively shielded from long-range interaction, that is, it occurs as if that interaction was absent. Shielding is a cooperative effect, because the time over which it is effective diverges with system size. In quantum systems, shielding can be related to the quantum Zeno effect. The latter refers to the confinement of the dynamics into invariant subspaces of a system under “continuous measurement”. This implies that long-range interaction plays a role similar to a measuring apparatus.

*

References

- [1] *Shielding and localization in the presence of long-range hopping.* , **G. L. Celardo**, R. Kaiser, and F. Borgonovi, Phys. Rev. B **94**, 144206 (2016).
- [2] *Cooperative Shielding in Many-Body Systems with Long-Range Interaction* , L. Santos, F. Borgonovi and **G.L.Celardo**, Phys. Rev. Lett. **116**, 250402 (2016).

Talk 28: Friday 17:30-18:30

**A fantasy about quasi 1D carbon molecules with decorations as
quantum registers**

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Poster 1: Wednesday 16:00-19:00

One-way ambipolar charge and valley transport in graphene bilayers

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First isolated in 2004 by Nobel Laureates Andre Geim and Konstantin Novoselov, graphene has united many record electrical, mechanical, thermal and optical properties (see for example [1]). The most notable electrical properties stem from its peculiar bandstructure which close to the Fermi energy combines a linear cone-like dispersion with pseudo-spin-momentum locking, similar to that expected for massless relativistic particles. There are two inequivalent cones in the energy dispersion, thereby leading to a binary spin-like flavor which is called the valley (see Fig. 1). The valley degree of freedom can be exploited for useful functions and may replace charge in low power applications.

A fundamental challenge is the formulation of a valley-controlled valley polarization source, in which the polarization of the valley degree of freedom can be flipped. This type of switchable valley source of electrons are the cornerstone for the future development of new valleytronics devices [2]. Here we explore the generation of charge and valley polarized unidirectional transport in graphene bilayers. With this aim we build on previous proposals [3, 4] and show how one-way ambipolar charge and valley transport can be achieved in graphene bilayers under experimentally feasible conditions.

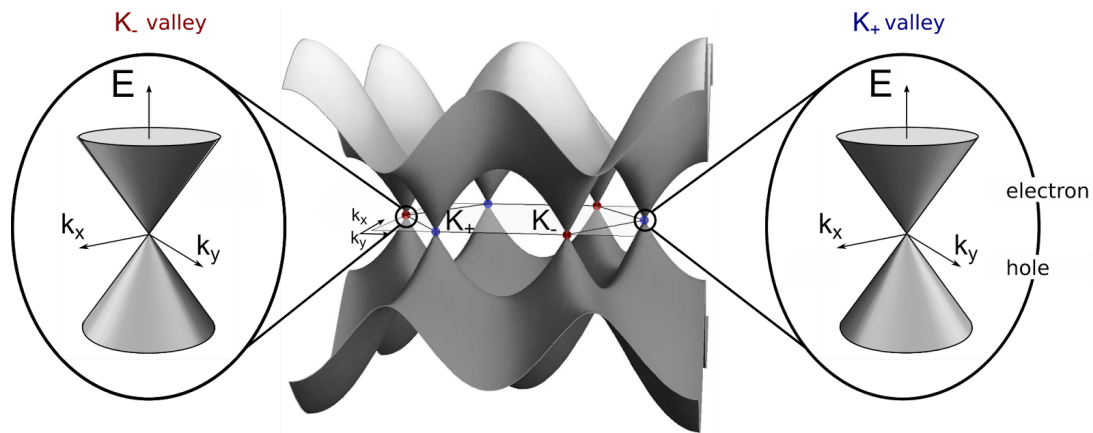


Fig. 1: Scheme showing graphene's band-structure obtained using the simplest tight-binding model. There are two inequivalent points in the Brillouin zone where the conduction and valence meet denoted with K_+ and K_- and which define the graphene "valleys". Adapted from Foa Torres, Roche, and Charlier, "Introduction to Graphene-Based Nanomaterials", Cambridge University Press 2014.

[1] Ferrari et al. *Nanoscale*, 7, 4598 (2015)

[2] J. R. Schaibley, H. Yu, G. Clark, P. Rivera, J. S. Ross, K. L. Seyler, W. Yao, X. Xu, *Nature Materials*, 1, 16055 (2016)

[3] L. E. F. Foa Torres, V. Dal Lago, E. Suárez Morell, *Phys. Rev. B*, 93, 075438 (2016)

[4] V. Dal Lago, E. Suárez Morell, L. E. F. Foa Torres, arxiv: 1708.03304

Poster 2: Wednesday 16:00-19:00

Transport and thermoelectric properties in periodic silicene superlattices

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Silicene is a monolayer of silicon atoms forming a two-dimensional low-buckled honeycomb lattice, which have received considerable attention in view of their attractive electronic and thermo-electronic properties (graphene-like) that promise potential applications for spintronic nano-devices. Silicene has a large intrinsic spin-orbit interaction and a buckled structure involving valley and spin manipulation (valley-spintronics). In this work, we have theoretically investigated the ballistic electronic transport and the thermoelectric effect of a periodic-potential structure in the monolayer silicene. The electronic transport properties like transmission and conductance are calculated by using the transfer matrix method. Also, we have studied the thermoelectric effect in this silicene structure by calculating the Seebeck coefficient and the thermopower factor, and their dependence for the spin-valley channels. We have found that the electronic transport and the thermoelectric properties can be modulated by the strength potential and the number of barriers of the superlattice structure.

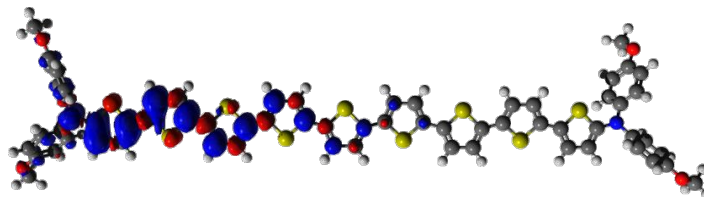
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Poster 3: Wednesday 16:00-19:00

Towards First-principles Evaluation of Transport Mechanisms in Molecular Wires

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Molecular wires are promising building blocks for electronic devices on the nanoscale as they offer the advantage of their miniaturization in comparison to the common silicone-based technology [1]. The charge transport in junctions comprising molecular wires is mainly described by two distinctly different mechanisms, coherent tunneling and incoherent hopping, where the molecular length is one of the key factors determining the governing mechanism as a transition from tunneling to hopping occurs upon elongation of the molecular bridge [2,3,4]. To evaluate how the transport mechanism can be predicted based on charge localization properties, several DFT approaches are validated regarding their performance of describing the degree of charge localization on the example of organic mixed-valence systems of different lengths with the aim of transferring them to predicting the experimentally observed charge transport mechanism in thiophene-based oligophenylene-imine wires [2] and guanine-based DNA sequences [5].

We show that a computational protocol based on the hybrid BLYP35 functional and a polarizable continuum model accounting for environmental effects, proposed by Kaupp and coworkers [6,7,8], provides a reasonable description of the length-dependent charge localization properties of organic mixed-valence systems on the borderline between full and partial charge localization in accordance with the experiment.

- [1] Heath, J. R.; Ratner, M. A. *Physics Today* **2003**, *56*, 43-49.
- [2] Smith, C. E.; Odoh, S. O.; Ghosh, S.; Gagliardi, L.; Cramer, C. J.; Christopher, J. K.; Frisbie, D. C., *J. Am. Chem. Soc.* **2015**, *137*, 15732-15741.
- [3] Zhao, X.; Huang, C.; Gulcur, M.; Batsanov, A. S.; Baghernejad, M.; Hong, W.; Bryce, M. R.; Wandlowski, T. *Chem. Mater.* **2013**, *25*, 4340-4347.
- [4] Cuevas, J. C.; Scheer, E. *Molecular Electronics: An Introduction to Theory and Experiment*. World Scientific, 2010.
- [5] Xiang, L.; Palma, J. L.; Bruot, C.; Mujica, V.; Ratner, M. A.; Tao, N. *Nat. Chem.* **2015**, *7*, 221-226.
- [6] Renz, M.; Kess, M.; Diedenhofen, M.; Klamt, A.; Kaupp, M. *J. Chem. Theory Comput.* **2012**, *8*, 4189-4203.
- [7] Renz, M.; Kaupp, M. *J. Phys. Chem. A* **2012**, *116*, 10629-10637.
- [8] Parthey, M.; Kaupp, M. *Chem. Soc. Rev.* **2014**, *43*, 5067-5088.

Poster 4: Wednesday 16:00-19:00

Efficient quantum transport in disordered interacting many-body systems

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Random matrices are popular models to represent interacting many-body systems in which disorder is an intrinsic property. We show measures for quantum transport in a disordered model (random matrix type) of interacting fermions which display efficient quantum transport. Our results generalize problems like the state transfer or the efficient quantum transport present in photosynthetic complexes.

Poster 5: Wednesday 16:00-19:00

Transfer Matrix Formalism for Heat Transport Problems

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The transfer matrix formalism is ubiquitous in the solution of transport and wave phenomena through periodic and aperiodic systems. Electron, phonon, wave propagation are some examples, and they have in common that their constitutive equations are hyperbolic.

The use of transfer matrices in heat transport problems has not developed and its main difference with other transport phenomena is the parabolic nature of the constitutive equation: Fourier's heat conduction law.

In this work, we present a general transfer matrix formalism for heat transfer by extending Fourier's law equation to an auxiliary Cattaneo hyperbolic equation [1] and constructing the transfer matrices for this type of equations. In the limit of instant response, Fourier's equation is recovered. Furthermore, we show that the formalism can easily be applied to different geometries.

As case study we present applications to simple layered superlattices [2], such as quantum wells, nested cylindrical systems like nanotubes [3] and finally to nested spherical shells. An important aspect of Cattaneo's equation is that it considers the finite response time of the system and its application to heating of nanostructures with ultrafast laser pulses [4]. The limitations of the technique when the phonons go from a ballistic to a diffusive regime will be discussed [5].

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[1] A. Compte and R. Metzler, *The generalized Cattaneo equation for the description of anomalous transport processes*, **30**, 7277 (1997).

[2] M. N. Luckyanova, J. Garg, K. Esfarjani, *Coherent phonon heat conduction in superlattices*, **338**, 936 (2012).

[3] G. Li, G. A. Lamberton and J. R. Gladden, *Acoustic modes of finite length homogeneous and layered cylindrical shells: Single and multiwall carbon nanotubes*. *J. Appl. Phys.* **104**, 033524 (2008).

[4] A. O. Govorov and W. Zheng, *Gold nanoparticles ensembles as heaters and actuators: melting and collective plasma resonances*, *Nanoscale Res. Lett.* **1**, 84 (2006).

[5] S. Volz (Ed.), *Microscale and Nanoscale Heat Transfer*, Topics in Applied Physics, vol. 107, Springer Verlag.

Poster 6: Wednesday 16:00-19:00

Electronic Properties of Polyacetylene and Polyethylene Molecules under the Effect of an External Electric Field

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Molecular electronics are being widely investigated because they are the next logical step in the miniaturization of electronic devices. The study of the electronic structure helps us to understand the conduction properties of the molecules to develop new devices specifically designed for our needs. Here, it is presented a computational study of the geometric and electronic structure of polyethylene and trans-polyacetylene. The calculations were performed using density functional theory and B3LYP/6-31+G* level. The molecules were studied in three different states: cationic, neutral and anionic, and it was studied the effect of an external electric field on the bond distance and molecular orbitals in each state. Results showed that the LUMO became localized because of the electric field. It was further examined the relationship between the localization of the orbitals and the size of the molecule. The relation of this electron localization with charge transport will be discussed.

Poster 7: Wednesday 16:00-19:00

High temperature induces order in unsupported graphene

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In this work we present a Raman study of supported and unsupported graphene as a function of temperature, from -180 °C to 800 °C. This study serves us to find a proper temperature interval to dope graphene. To this end, we obtain graphene by chemical vapor deposition technique at atmospheric pressure [1]. After the synthesis, graphene is translated on the different substrates for Raman characterization. Silicon substrate was used for supported graphene, TEM Au grids and graphite flakes with holes for unsupported graphene. We found that using graphite flakes with holes it was possible to achieve 800 °C without damage in graphene, while using TEM Au grids we only could heat the sample at 500 °C. From 25°C to 400 °C D peak is so strong in intensity and the most important finding is that at 500 °C this peak of graphene disappears. Therefore we believe that using these findings it will be possible to use thermal treatments to dope graphene in two stages, first at 400 °C to absorb dopants atoms and then 600 °C to ensure a strong bond between carbon and dopants. Also we performed transport measurements to characterized the samples using this new method.

References:

[1] C. Bautista Flores, et al. Chem. Phys. Lett. **665** (2016), 121-126.

Poster 8: Wednesday 16:00-19:00

Title: Comparison of charge transmission for graphene and silicene in self-similar structures.

Author: Díaz Guerrero Dan Sidney.

Abstract

In the past few years it has been discovered that charge transmission in self-similar structures for graphene have scaling rules between transmission curves. The transfer matrix method was applied to obtain the transmission coefficient, and due to the nature of the method it was not been possible to deduce the scaling rules analytically. So in order to unveil the particular properties of self-similar structures based on graphene comparisons has been made with gallium arsenide. Nevertheless it is appealing to compare it with other two-dimensional materials.

Among the two-dimensional materials silicene is the one considered in this work due to its dominance in the electronic components of today. The first task is to search for scaling rules in the charge transmission for self-similar structures based on silicene. Then if such rules exist compare their expression with those corresponding to graphene. It would expected that if indeed there are scaling rules in the transmission for self-similar structures based on silicene they should be very different from the ones found for graphene. In either case, that is if they are different or not, this should help to distinguish the contribution of the self-similar structures over the scaling rules and the contribution of the material intrinsic properties.

Poster 9: Wednesday 16:00-19:00

Efficient Calculation of Electron-Phonon Coupling in Molecular Junctions

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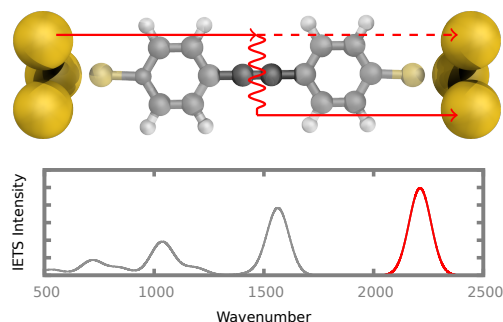
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Electron transport through individual molecules is important for many biological processes and potential technological applications. Great experimental and theoretical progress in this field in recent years also provides insight into molecular junctions under unusual (nonequilibrium) conditions. Aside from elastic processes, inelastic ones such as the excitation of spin flips or vibrations can occur. The strength of the latter is dominated by the electron-phonon coupling and is experimentally studied within the framework of inelastic electron tunneling spectroscopy using break junctions or scanning tunneling setups [1].

The challenging aspect for theory is the sensitivity of the IET spectrum to minor changes of the molecule or the environment such as the junction geometry [2, 3]. Thus, efficient ways to study several junctions or structure–property relations are needed.

To provide an efficient framework for calculating IET spectra, we combine the mode-tracking algorithm (an iterative subspace approach for selectively calculating eigenvectors and -modes of the Hessian matrix) as implemented in MoViPaC [4, 5, 6] with our program package ARTAIOS [7, 8]. We show a variety of calculated spectra, compare them with experimental data and demonstrate the capabilities of our mode-tracking approach by e.g. showing results for different numbers of gold atoms included in the electrodes.



- [1] M. A. Reed, *Materials Today* **2008**, *11*, 46–50.
- [2] M. Kula, J. Jiang, Y. Luo, *Nano Lett.* **2006**, *6*, 1693–1698.
- [3] R. Frisenda, M. L. Perrin, H. S. J. van der Zant, *Beilstein Journal of Nanotechnology* **2015**, *6*, 2477–2484.
- [4] T. Weymuth, M. P. Haag, K. Kiewisch, S. Luber, S. Schenk, C. R. Jacob, C. Herrmann, J. Neugebauer, M. Reiher, *Journal of Computational Chemistry* **2012**, *33*, 2186–2198.
- [5] M. Reiher, J. Neugebauer, *The Journal of Chemical Physics* **2003**, *118*, 1634–1641.
- [6] C. Herrmann, J. Neugebauer, M. Reiher, *New Journal of Chemistry* **2007**, *31*, 818.
- [7] C. Herrmann, G. C. Solomon, J. E. Subotnik, V. Mujica, M. A. Ratner, *The Journal of Chemical Physics* **2010**, *132*, 024103.
- [8] M. Deffner, L. Gross, T. Steenbock, B. A. Voigt, G. C. Solomon, C. Herrmann, “ARTAIOS - a transport code for postprocessing quantum chemical electronic structure calculations, available from <https://www.chemie.uni-hamburg.de/ac/herrmann/software/index.html>”, 2009–2017.

Poster 10: Wednesday 16:00-19:00

Cooperativity and scalability of light-harvesting devices by decoupling absorption from transmission

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Engineering devices able to exploit quantum features at room temperature is one of the main challenges in quantum technologies related to basic energy science and quantum sensing. In natural photosynthetic systems extended exciton states are thought to play a fundamental functional role, inducing cooperative coherent effects, such as super-absorption of light and super-transfer of excitation. One of the main limitations of light-harvesting devices lies in the fact that super-absorption of light is often accompanied with super-emission. The time reversal nature of such processes greatly limit the scalability of the devices, inducing a saturation of their efficiency above a critical system size. In order to avoid such limitations, here we design a bio-inspired light-harvesting/photon sensing device where the absorbing states lies in the upper part of the spectrum while transferring states lies in the lower part. Decoupling is achieved exploiting the fast thermal relaxation which brings the excitation from the high energy absorbing state to the low energy transmitting states before emission occurs. The proposed model consists of a ring of donors surrounding a central core absorber, under the combined action of a polarized laser field and a thermal bath. The working principle of this device is based on three step:

- i) super-absorption of light from high energy states,
- ii) thermal relaxation which drives the excitation to low energy states,
- iii) optimal transfer of the excitation from low energy states to the central core absorber.

While in many relevant natural complexes absorbing and transferring states are the same, such device is based on the decoupling of absorption and transfer. Here we show that such decoupling greatly improve the efficiency and the scalability of the system, indeed we show that the saturation of their efficiency occurs for much larger system size.

Poster 11: Wednesday 16:00-19:00

Topological flat bands in time-periodically driven uniaxial strained graphene nanoribbons

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We study the emergence of electronic nontrivial topological flat bands in time-periodically driven strained graphene within a tight-binding approach based on the Floquet formalism. In particular, we focus on uniaxial spatially periodic strain since it can be mapped onto an effective one-dimensional system. Also, two kinds of time-periodic driving are considered: a short pulse (delta kicking) and a sinusoidal variation (harmonic driving). We prove that for special strain wavelengths, the system is described by a two-level Dirac Hamiltonian. Even though the study case is gapless, we find that topologically nontrivial flat bands emerge not only at zero-quasienergy but also at $\pm\pi$ quasienergy, the latter being a direct consequence of the periodicity of the Floquet space. Both kind of flat bands are thus understood as dispersionless bands joining two inequivalent touching band points with opposite Berry phase.

Poster 12: Wednesday 16:00-19:00

Magneto-optical conductivity of strained graphene

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We report an analytical study on the optical response of strained graphene in the presence of an external magnetic field. From Kubo formalism, the magneto-optical conductivity of strained graphene is obtained within Dirac approximation. Such conductivity results a tensor neither symmetric nor antisymmetric. We analyze the combined effects of strain-induced anisotropy and magnetic field on the transmittance as well as on the Faraday rotation of linearly polarized light after passing through the strained graphene. Moreover, we provide a generalized expression of the Faraday angle, which allows to identify the strain-induced effects as in comparison to the magnetic effects. Finally, our findings for strained graphene are extended to anisotropic two-dimensional materials with massless Dirac fermions of arbitrary pseudospin.

Poster 13: Wednesday 16:00-19:00

Self-similar transport in graphene: The role of magnetic field effects and breaking-symmetry substrates

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Recently, it has been reported that the electron transport in graphene manifests self-similar characteristics once the graphene sheet is nanopatterned with special geometries like those based on the Sierpinski carpet and the Cantor set [1,2]. The 2D nature of graphene, the quantum relativistic character of Dirac electrons as well as the nanopatterned complex geometry give rise to this peculiar phenomenon of self-similar transport in graphene. As far as we know self-similar transport constitutes another exotic transport phenomenon in graphene because there is no other material in which the complex geometrical features impact directly in physical measurable properties. Here, we examine the transport properties when the graphene sheet is nanopatterning with external magnetic fields and breaking-symmetry substrates in Cantor-like fashion. We find that magnetic field effects induce self-similar patterns in the transmission properties with well defined scaling mathematical expressions. In the case of breaking-symmetry substrates the transmission as well as the transport properties manifest self-similar characteristics. As a final comment, it is important to remark that it seems fundamental to break some symmetry of graphene in order to obtain self-similar transport. In the case of the magnetic field the time reversal symmetry is broken, while for substrates the graphene's sublattices symmetry is not preserved.

1. E. Van Veen, S. Yuan, M. I. Katsnelson, M. Polini, A. Tomadin, Phys. Rev. B **93**, 115428 (2016).
2. H. García-Cervantes, L. M. Gaggero-Sager, D. S. Díaz-Guerrero, O. Sotolongo-Costa, I. Rodríguez-Vargas, Scientific Reports **7**, 617 (2017).