Graphene Day: October 11, salle Itzykson, SPEC/CEA Saclay

Organizers: Preden Roulleau and Simon Vassant

9h50 – 10h: Introduction (Preden Roulleau)

10h-10h30: Bernard Plaçais, *Landau velocity for collective quantum Hall breakdown in bilayer graphene*

10h30-11h00: Taro Wakamura, *Strong Anisotropic Spin-Orbit Interaction in Graphene Induced by Transition Metal Dichalcogenides*

11h00-11h20: *Coffee Break*

11h20-11h50: Fabrice Charra, *Photonic properties of graphene-based 2D supramolecular self-assembled architectures*

11h50- 12h20: Sylvain Latil, *Optical properties in hexagonal Boron Nitride: the influence of the atomic structure.*

12h20 – 14h00: *Lunch Break*

14h00 -14h30: François Parmentier, *Quantum transport in graphene in SPEC: CVD, SiC, vdW*

14h30 – 15h: Christophe Voisin, *hyperbolic cooling of hot electrons in a BN supported graphene transistor.*

15h00 -15h20: *Coffee Break*

15h20 – 15h50: Yannick Dappe, *Density Functional Theory as a tool to study graphene and 2D materials: application to gap modulation in graphene based van der Waals heterostructures*

15h50 – 16h20: Cyrille Barreteau, *A bird's eye view on the flat and conic band world of the honeycomb and Kagome lattices: towards an understanding of 2D metal-organic frameworks electronic structure*

16h20 – 16h40: *Discussions*

Landau velocity for collective quantum Hall breakdown in bilayer graphene

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Breakdown of the quantum Hall effect (QHE) is commonly associated with an electric field approaching the inter Landau-level (LL) Zener field, ratio of the Landau gap and cyclotron radius. Eluded in semiconducting heterostructures, in spite of extensive investigation, the intrinsic Zener limit is reported here using high-mobility bilayer graphene and high-frequency current noise [1,2]. We show that collective excitations arising from electron-electron interactions are essential. Beyond a noiseless ballistic QHE regime a large superpoissonian shot noise signals the breakdown via inter-LL scattering [1]. The breakdown is ultimately limited by collective excitations in a regime where phonon and impurity scattering are quenched. The breakdown mechanism can be described by a Landau critical velocity as it bears strong similarities with the roton mechanism of superfluids. In addition we show that breakdown is a precursor of an electric-field induced QHE-metal transition.

[1] Yang et al., Phys. Rev. Lett., accepted Sept. 4th. 2018
[2] Yang et al., Nat. Nanotech. 13, 47 (2018).

Strong Anisotropic Spin-Orbit Interaction in Graphene Induced by Transition Metal Dichalcogenides

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Graphene is known as an ideal material for the long spin coherent transport owing to its small spin-orbit interaction (SOI). However, the conventional spin injection method by using ferromagnetic (F) electrodes suffers the impedance mismatch problem between graphene and F metals, and these F electrodes also cause spin-flip scatterings which limit ideal long spin coherence. Since spin currents can also be created via the spin Hall effect (SHE), enhancing SOI in graphene is a crucial step to realize the generation of spin currents in graphene by itself. SOI is also an essential building block for the topological phenomena, and it can drive graphene into the two-dimensional (2D) topological insulator (quantum spin Hall (QSH) insulator). Therefore generation of strong SOI in graphene is an important task to progress research on both spintronics and topological physics.

In this study, we demonstrate strong SOI in graphene induced by transition metal dichalcogenides (TMDs). TMDs are two dimensional materials similar to graphene, and they have strong intrinsic SOI due to heavy transition metal elements. Interestingly, they have different band structures depending on the thickness. We fabricated heterostructures with graphene and WS_2 by using both monolayer and bulk WS_2 to investigate the difference between them in the capacity to induce SOI in neighboring graphene.

To evaluate the amplitudes of the induced SOI in graphene, we performed magneto-transport measurements at low temperatures. While pristine graphene exhibits the weak localization behavior due to the small SOI, graphene on both monolayer and bulk WS_2 show weak antilocalization peaks, a signature of the strong SOI induced in graphene. Surprisingly, the observed magnetoresistance curves show drastically different shapes between the graphene/monolayer and graphene/bulk WS_2 samples. The detailed analysis based on the theoretical formula demonstrates that the induced SOI in graphene is much stronger for graphene/monolayer WS_2 samples than for graphene/bulk WS_2 ones.

We also investigated the symmetry of the induced SOI. The dominant mirror-symmetric SOI with graphene as a mirror plane is essential to realize the QSH state, thus it is significant to scrutinize the symmetry of the induced SOI. From the theoretical fits of the magneto-transport data, we found that symmetric SOI is much more dominant than the asymmetric one. The symmetric SOI in this system is composed of the two contributions, the intrinsic SOI and valley-Zeeman SOI, a unique type of SOI in this system. To determine the dominant type of the SOI in the symmetric contribution, we analyzed the spin relaxation mechanisms. In graphene, the two spin relaxation mechanisms, the Elliot-Yafet (EY) and D'yakonov-Perel mechanisms are possible. The former is caused by the intrinsic SOI, and the latter relevant to the valley-Zeeman (VZ) SOI. From the analysis we found that the EY contribution is dominant close to the Dirac point. This result indicates the existence of the intrinsic SOI, essential to realize the QSH state. Our findings on introduction of SOI in graphene reveal that graphene can be a promising material for both spintronics and topological physics [1,2].

[1] T. Wakamura *et al*., Phys. Rev. Lett. **120**, 106802 (2018).

[2] T. Wakamura *et al*., arxiv:1809.06230.

Photonic properties of graphene-based 2D supramolecular self-assembled architectures

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Graphene is a zero band-gap semiconductor, which confers to it many remarkable and potentially exploitable optoelectronic properties. The modulation of these properties, which can be obtained by molecular functionalization, is an important current issue for such applications. We have recently developed original molecular-engineering concepts for designing molecular building blocks spontaneously adsorbing on graphene according to various preprogrammed patterns.[1] We have realized and probed the photonic responses of several self-assembled molecular or polymeric structures grown onto graphene. The STM images permit an accurate structural analysis of molecular organization induced by the atomic-scale template of graphene.[2] The organized self-assembly has a clear influence on optical properties, as observed by transmission and fluorescence spectroscopy.[3,4] We also report the first fluorescent molecular self-assembly on graphene.[5] The inherent quenching of excited-state by the adjacent graphene is hindered at the molecular scale based on a spacer approach, through specifically designed dual-functionalized self-assembling building blocks.

[1] G. Schull et al, Nanolett, 6, 1360-1373 (2006)
[2] N. Kalashnyk et al, Chem. Commun., 54, 9607-9610 (2018)
[3] T. Sghaier et al, Beilstein J. Nanotechnol. 7, 862-868 (2016)
[4] S. Le Liepvre et al, Mol. Cryst. Liq. Cryst. 65, 5-15 (2017)
[5] S. Le Liepvre et al, ACS Photonics 3, 2291-2296 (2016)

OPTICAL PROPERTIES IN HEXAGONAL BORON NITRIDE: THE INFLUENCE OF THE ATOMIC STRUCTURE

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Layered hexagonal boron nitride (hBN) is a wide band gap semiconductor (> 6 eV) which attracts a growing interest for its strong UV photo-luminescence properties [1]. The optical properties of bulk hBN as well as BN layers are governed by strong excitonic effects. They have been studied recently, but experiments are difficult because of the necessity to work in the far UV range [2].

We address this issue from the theoretical point of view by combining many body perturbation theory (GW approximation and Bethe-Salpeter equation) and tight-binding model. In case of the monolayer, we present a detailed theoretical study of the first excitonic levels, and characterize their energies and shape [3]. Strong deviations from the usual hydrogenoic model are evidenced due to both lattice effects and the 2D nature of the screening, which can be approximated by a potential of the Keldysh shape.

In a second time, we focus on the exciton dispersion rather than the single-particle band structure to investigate the excitonic properties of the monolayer and of some bulk polymorphs of hBN, with the intent of disclosing the connections between atomic arrangement, single-particle band structure and exciton dispersion [4].

References

[1] L. Wirtz et al., *Phys. Rev. Lett*. **96** 126104 (2006).
[2] L. Schué et al., *Nanoscale* **8**, 6986 (2016).
[3] T. Galvani et al., *Phys. Rev. B*. **94**, 125303 (2016).
[4] L. Sponza et al., arXiv :1806.06201.

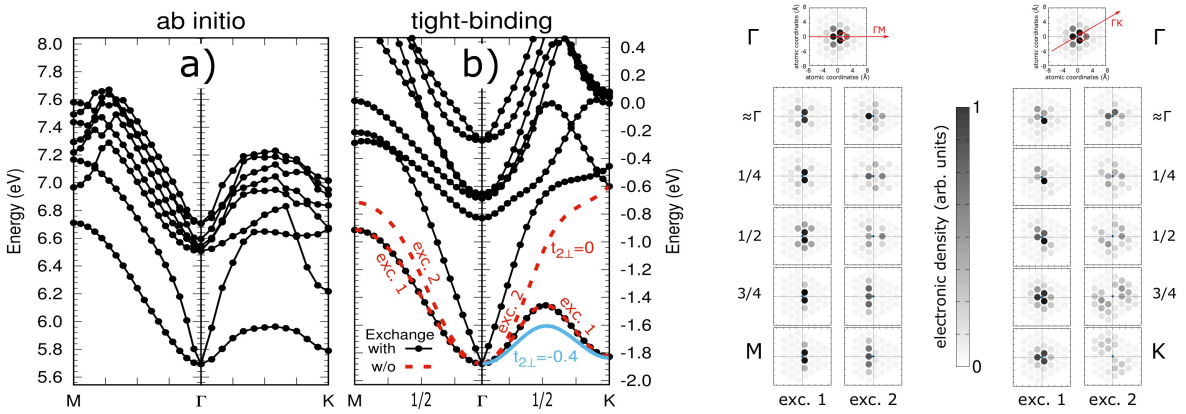

Figure : At left: ab initio (a) and tight-binding (b) dispersions of excitons in hBN for q vector along the ΓMK path. At right: tight-binding spatial representation of the (electronic) density for the first two excitons. The hole is located at the centre.

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Quantum transport in graphene in SPEC: CVD, SiC, vdW

François Parmentier, SPEC/CEA Saclay

Raising the quality of graphene samples allows uncovering increasingly subtle and fundamental properties of electronic quantum transport in this material. I will review the various graphene experiments realized in the Nanoelectronics group of SPEC in the past years, emphasizing how developing and implementing state-of-the-art fabrication techniques allowed us to further explore mesoscopic physics in graphene. In particular, the quantum Hall effect shows dramatically new and exciting features when going from high quality epitaxial graphene on silicon carbide to ultra-high quality, modular van der Waals heterostructures, where graphene flakes are encapsulated between atomically flat boron nitride crystals.

HYPERBOLIC COOLING OF HOT ELECTRONS IN A BN SUPPORTED GRAPHENE TRANSISTOR.

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Power dissipation is a key issue in nano-electronics. In particular, the future of graphene transistors lies in radio-frequency (RF) power amplification in the saturation regime [1]. In this high-bias regime the power to be dissipated becomes considerable and a good understanding of the thermal conductance mechanisms is essential for future developments. Here, we consider the case of BN-supported graphene devices that are known to bring the best mobilities required to reach the saturation regime. In this case, the usual dissipation channels related to acoustic phonons or impurity scattering are suppressed, bringing up an original scenario where the electrons are strongly decoupled from the lattice.

In this work, we drive the transistor far from equilibrium by applying a strong DC bias leading to Joule self-heating of the electrons. The electron temperature is monitored by noise thermometry (Johnson-Nyquist noise) in the 0-10GHz band [2]. By increasing the injected power, we first observe a quadratic behavior typical of the (inefficient) electronic heat conduction to the leads (Wiedeman-Franz regime). Nevertheless, above a doping dependent threshold, the electronic temperature eventually levels off at plateaus of several thousands of Kelvin (Figure 1) where the power dissipation is in the range of 10^9 W.m^{-2} [3].

This striking behavior is explained quantitatively by the coupling of hot electrons with the hyperbolic phonon polaritons of the BN supporting layer [3]. These modes arise in the reststrahlen bands of BN at 80~meV and 160 meV and make up for a very efficient conduction channel as long as the hot electron bath is located in their near field, which is the case in our geometry. The switching on of this channel is triggered by the doping dependent mode matching between the optical conductance of graphene and the optical admittance of the BN layer (Figure 2).

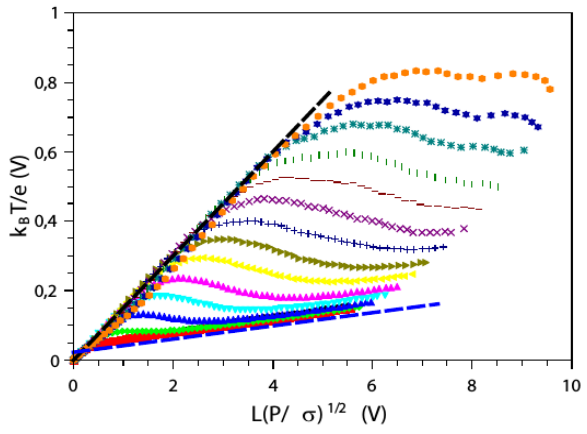

Figure 1 : Experimental steady state electronic temperature in a BN supported bilayer graphene transistor as a function of the (square root of) the injected power

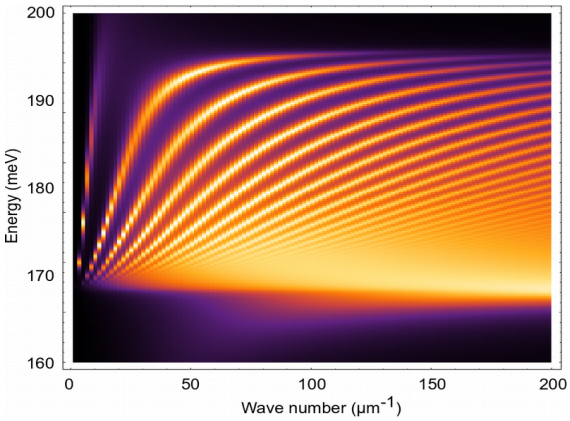

Figure 2 : Computed mode matching function of a bilayer graphene on a 23nm thick BN layer on gold showing strong matching with the hyperbolic modes (Ef=100meV, Te=1000K).

References

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[2] A. Betz *et al.*, Phys. Rev. Lett. **109**, 056805 (2012), Nat. Phys. **9**, 109 (2013)

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Density Functional Theory as a tool to study graphene and 2D materials: application to gap modulation in graphene based van der Waals heterostructures

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The possibility of isolating one monolayer of graphene in 2004 has opened a wide field of research in the study of bidimensional (2D) materials. In particular, the vertical stacking of different 2D materials, like graphene, hexagonal boron-nitride (hBN) or Transition metal dichalcogenide (TMD), called van der Waals (vdW) heterostructures, offers promising perspectives for future nanoelectronics. Hence, as stated by Geim and Grigorieva [1], due to the weak vdW interaction between the different layers, the vertical stacking of those materials results in the superposition of the different electronic structures through Fermi level alignment. Consequently, many experimental studies have been devoted to the combination of different 2D materials in various vdW heterostructures. In that respect, Density Functional Theory (DFT) represents an important theoretical support in order to fully interpret the obtained experimental data as well as to predict new phenomena to be tested experimentally. In this presentation, I will show some results obtained in DFT in collaboration with experiments, in particular on the gap modulation in a bilayer graphene stacked between a substrate and a TMD [2,3]. Besides this specific example, I will stress the quantities that can be extracted from DFT calculations to be compared with experimental data or to be used for Physical models in the understanding of 2D materials.

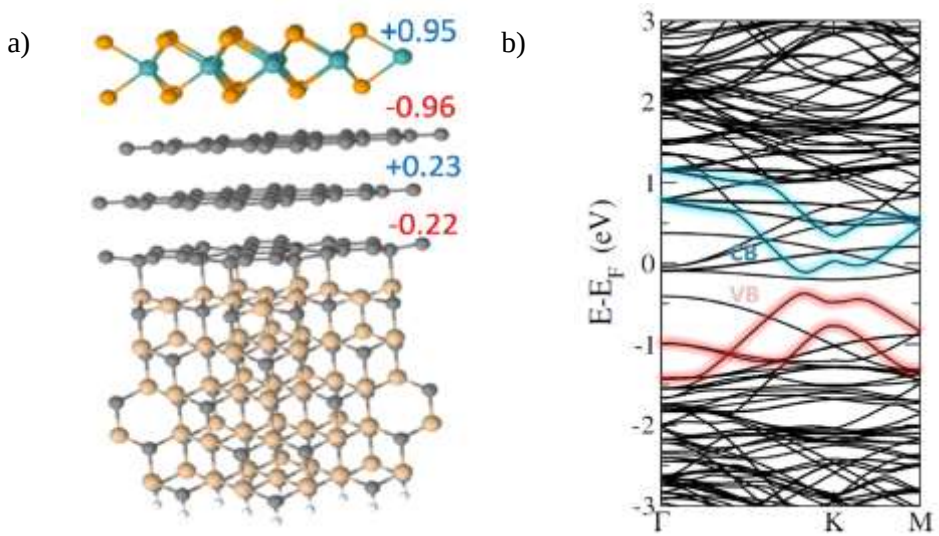

Figure 1: a) Atomic representation of a typical unit cell for DFT calculations of a $MoSe_2$/bilayer graphene/SiC heterostructure with indication of the corresponding electronic charges. b) Corresponding electronic bandstructure calculated in DFT with indication of the electronic gap in the bilayer graphene.

References

[1] A.K. Geim and I.V. Giregorieva, *Nature* **499**, 419 (2013).

[2] M.T. Dau *et al*, *ACS Nano* **12**, 2319 (2018).

[3] D. Pierucci *et al*, *NanoResearch* **8**, 1026 (2015).

A bird's eye view on the flat and conic band world of the honeycomb and Kagome lattices: towards an understanding of 2D metal-organic frameworks electronic structure

Cyrille Barreteau (SPEC), François Ducastelle (ONERA), Talal Mallah (ICMMO)

I will present an electronic structure analysis of a wide variety of lattices belonging to the class of honeycomb and Kagome systems including several mixed forms combining both lattices. The band structure of these systems are made of a combination of dispersive and flat bands. The dispersive bands possess Dirac cones (linear dispersion) at the six corners (K points) of the Brillouin zone, although in some peculiar cases Dirac cones can also appear at the center of the zone (Gamma point). The flat bands can be of different natures. Most of them are tangent to the dispersive bands at the center of the zone but some, for symmetry reasons, do not hybridize with other bands. These types of lattices are encountered in various systems such as metal-organic frameworks (MOF), semiconductor nanocrystals or photonic crystals. The objective of our work is to provide a thorough analysis of a wide class of so-called ligand-decorated honeycomb Kagome lattices that are observed in a 2D MOF where the ligand occupy honeycomb sites and the metallic atoms the Kagome sites.