NANOSIM_GRAPHENE

Simulation of Graphene-based Nanomaterials and Nanodevices : Multiscale Approaches

Call : ANR-P3N 2009 Period : 4 ans (2010 – 2013)

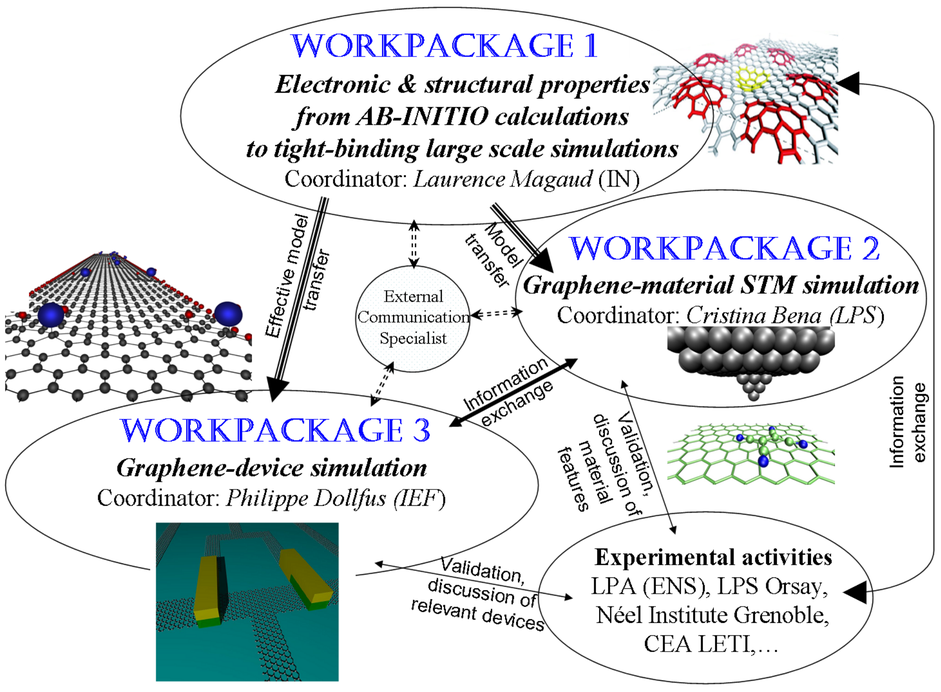
Summary : The purpose of NANOSIM_GRAPHENE is to establish a multi-scale simulation methodology of graphene-based nanomaterials and nanodevices. Graphene is a two-dimensional monolayer of sp^2 bonded carbon atoms in a dense honeycomb crystal structure which behaves electronically as a zero-gap semiconductor. Exceptional electronic properties of this material, resulting for instance in carrier mobilities as large as several thousands of cm^2/Vs, make this material a main driver of the beyond-CMOS nanoelectronics research. A key issue lies however in the strategy to design graphene-based materials with enhanced energy (or transport) gap, allowing for field effect efficiency and device capability. In this respect, the chemical complexity of graphene demands in-depth quantum simulation analysis for understanding of the material properties and further optimization of graphene-based device performance.

Partners :

- CEA INAC and LETI → quantum transport and *ab initio* simulation
- IEF Orsay → quantum transport with electron-phonon coupling
- Institut Néel Grenoble → *ab initio* (substrate, interfaces)
- IMN Nantes → *ab initio* (defects, impurities, functionalization)
- LPS Orsay → fundamental aspects of the electronic structure
- Nanotimes → Simulation for Scanning tunneling microscopy

Collaborations :

- Ecole Polytechnique de Montréal
- Hanoi Advanced School of Science and Technology
- Institut Català de Nanotecnologia (ICN)

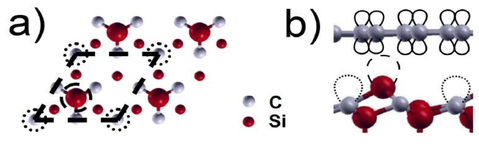


WP 1: Electronic & Structural Properties

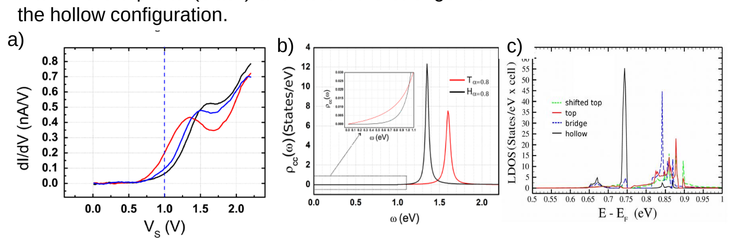
Graphene – Defect interaction

We take advantage of the peculiar geometry of graphene on the C face of SiC in the (2x2) reconstruction to investigate graphene – defect interaction as a function of local stacking. We compare STM experiments to ab initio calculations and results obtained within the Anderson model.

The three approaches give similar trends : resonance due to defect is much sharper in the hollow site (red) than in the top site (black) and its shift is stronger for the hollow configuration.



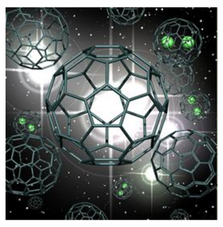
Graphene on C face of SiC. a) (2x2) reconstruction of the free SiC surface, b) graphene on top of SiC



DOS on the defect : a) STM dI/dV, b) Anderson's model c) ab initio calculation of the true interface geometry.

DFT modelling of fullerene closed-cage growth, a first step to understanding carbon incorporation into sp^2-based nanocarbon networks

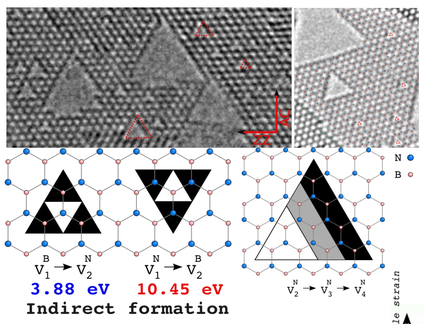
In the last half of 2011 / start of 2012 we have made in-roads into computer modelling of carbon growth processes, focussing some effort on understanding the growth processes of carbon fullerenes – the oldest and best understood of the carbon nanomaterials. It is hoped that insights into the growth procedure for these molecules will be transferable to high-temperature graphene growth. In collaboration with experimental colleagues at Florida State University we were able to show unambiguously a closed-cage growth mechanism for fullerenes, via incorporation of C and C_2 moieties. The results were published in Nature Communications [1] and received significant press coverage (e.g. Chemistry World [2]).



[1] 'Closed network growth of fullerenes', P. W. Dunk, N. K. Kaiser, C. L. Hendrickson, J. P. Quinn, C. P. Ewels, Y. Nakanishi, Y. Sasaki, H. Shinohara, A. G. Marhsall, H. W. Kroto, Nature Communications 3, 856 (2012)
[2] 'Buckyballs grow by gobbling up carbon', Chemistry World, May 2012,
http://www.rsc.org/chemistryworld/2012/05/buckyballs-grow-gobbling-carbon

h-BN : Triangular multivacancies with N-terminated zigzag edges

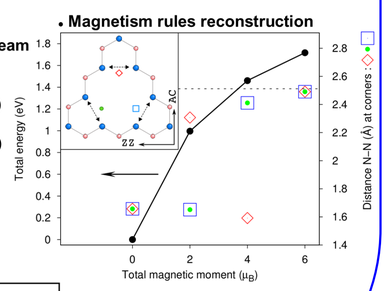
§ ***Approach***: BiGDFT (450 atoms)



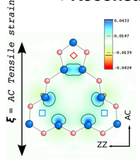
V_t	V^B (eV)	V^N (eV)
1	8.17	6.71
2	17.16	12.05
3	23.96	19.93

Direct formation

• **Magnetism rules reconstruction**



• **Reconstruction rules magnetism**



0 % < ξ < 2.0%	M = 0 μB
2.0 % < ξ < 3.0%	M = 4 μB
ξ > 3.0%	M = 0 μB

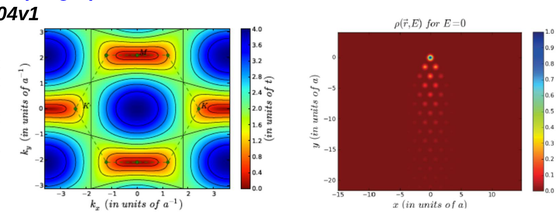
§ Appl. Phys. Lett. **101**, 132405 (2012)

WP 2: Graphene-material STM simulation

Friedel oscillations at the Dirac-cone-merging point in anisotropic graphene

C. Dutreix, L. Bilteanu, A. Jagannathan, C. Bena, ***arXiv:1210.5104v1***

We have studied the Friedel oscillations induced by a localized impurity in anisotropic graphene. We have focused on the limit when the two inequivalent Dirac points merge. We have found that in this limit the Friedel oscillations manifest very peculiar features, such as a strong anisotropy and an atypical inverse square-root decay. Our calculations have been performed using both a T-matrix approximation and a tight-binding exact diagonalization technique. They have allowed us to obtain numerically the local density of states as a function of energy and position, as well as an analytical form of the Friedel oscillations in the continuum limit. The two techniques yield results that are in excellent agreement, confirming the accuracy of such methods to approach this problem.



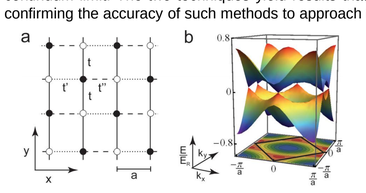


FIG. 1: (color online). (a) Square lattice indicating the hopping amplitudes and the two inequivalent sites. (b) Band structure in the gapless D phase for $t' = t = 0.2$, $t'' = 0.05$ in units of E_R, see text. The first Brillouin zone is indicated by the square.

Bloch-Zener oscillations across a merging transition of Dirac points,

Lih-King Lim, Jean-Noël Fuchs, Gilles Montambaux,
Phys. Rev. Lett. 108, 175303 (2012)

Bloch oscillations are a powerful tool to investigate spectra with Dirac points. By varying band parameters, Dirac points can be manipulated and merged at a topological transition towards a gapped phase. Under a constant force, a Fermi sea initially in the lower band performs Bloch oscillations and may Zener tunnel to the upper band mostly at the location of the Dirac points. The tunneling probability is computed from the low energy universal Hamiltonian describing thevicinity of the merging. The agreement with a recent experiment on cold atoms in an optical lattice is very good.

Magnetic spectrum of trigonally warped bilayer graphene: semiclassical analysis, zero modes, and topological winding numbers

R. de Gail, M. O. Goerbig, G. Montambaux, ***Phys. Rev. B 86, 045407 (2012)***

We have investigated the fine structure in the energy spectrum of bilayer graphene in the presence of various stacking defaults, such as a translational or rotational mismatch. This fine structure consists of four Dirac points that move away from their original positions as a consequence of the mismatch and eventually merge in various manners. The different types of merging are described in terms of topological invariants (winding numbers) that determine the Landau-level spectrum in the presence of a magnetic field as well as the degeneracy of the levels. The Landau-level spectrum is, within a wide parameter range, well described by a semiclassical treatment that makes use of topological winding numbers. However, the latter need to be redefined at zero energy in the high-magnetic-field limit as well as in the vicinity of saddle points in the zero-field dispersion relation.

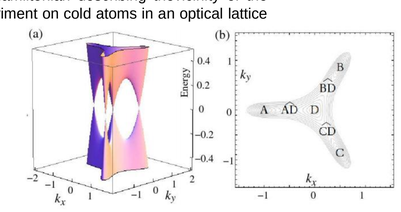


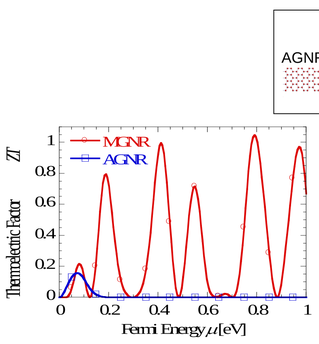
FIG. 2. (Color online) (a) Band structure of the perfectly AB-stacked bilayer graphene around one of the valleys. (b) Position of the remarkable points in reciprocal space. We label the four Dirac cones from A to D and the corresponding saddle points $\widehat{AD}$, $\widehat{BD}$ and $\widehat{CD}$. While the Dirac points all reside at zero energy, the saddle points have an energy $E = c^2/4b$. The wave vectors are measured in units of c/b and the energy in units of c^2/b.

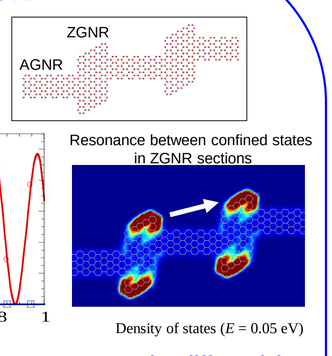
WP 3: Graphene device simulation

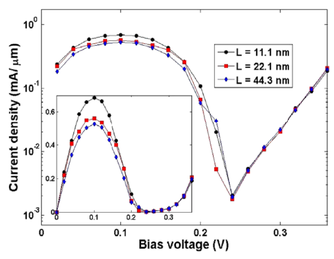
Enhanced thermoelectric properties in graphene nanoribbons by resonant tunneling of electrons

F. Mazzamuto, V. Hung Nguyen, Y. Apertet, C. Caër, C. Chassat, J. Saint-Martin, P. Dollfus, Phys. Rev. B 83, 235426 (2011)

By means of NEGF atomistic simulation of electron and phonon transport, we analyze the thermal and electrical properties of perfect GNRs as a function of their width edge orientation to identify a strategy likely to degrade the thermal conductance while retaining high electronic conductance and thermopower. An effect of resonant tunneling of electrons is detected in mixed GNRs consisting of alternate zigzag and armchair sections. A structure with armchair and zigzag sections of different widths is shown to provide a high thermoelectric factor of merit *ZT* exceeding unity at room temperature.







Graphene nanomesh-based devices exhibiting a strong negative differential conductance effect

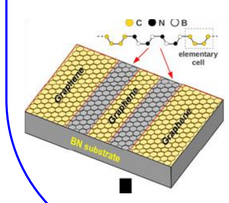
V. Hung Nguyen, F. Mazzamuto, J. Saint-Martin, A. Bournel, P. Dollfus, Nanotechnology 23 (2012) 065201

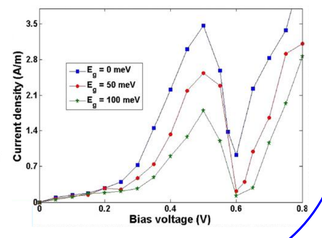
We have investigated the transport characteristics of graphene nanomesh-based devices and evaluated the possibilities of observing negative differential conductance. By taking advantage of bandgap opening in the graphene nanomesh lattice, a strong negative differential conductance effect can be achieved at 300K in pn junctions and n-doped structures. Remarkably, the effect is improved very significantly (with a peak-to-valley current ratio of a few hundred) and appears to be weakly sensitive to the transition length in graphene nanomesh pn hetero-junctions when inserting a pristine (gapless) graphene section in the transition region between n and p zones. It suggests new strategies for graphene electronic devices which may offer strong advantages in terms of performance and processing over the devices studied previously.

Resonant tunneling diode based on graphene/h-BN heterostructure

V. Hung Nguyen, F. Mazzamuto, A. Bournel, P. Dollfus, J. Phys. D 45 (2012) 325104

we propose a resonant tunnelling diode (RTD) based on a double-barrier graphene/BN heterostructure as a device suitable to take advantage of the elaboration of atomic sheets containing different domains of BN and C phases within a hexagonal lattice. The device operation and performance are investigated by means of a self-consistent solution within the NEGF formalism on a TB Hamiltonian. This RTD exhibits a negative differential conductance effect, which involves the RT through both the electron and hole bound states in the graphene quantum well. The peak-to-valley ratio reaches 4 at 300K even for zero bandgap and can be higher than 10 when a finite gap opens in the graphene channel.





Project outcome and impact in 2011-2012:

- 1 book chapter + 25 papers including in PRL, APL, PRB, Nature Naotechnology
- 10 invited and keynote talks including at Carbon, Graphene2012, GRIMM3, STEG
- 2 Invited lectures including ENSICAEN and Cargese Int. School
- 25 contributed talks and posters
- Active involvement in Lavoisier Discussions and preparation of EU Graphene Flagship

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