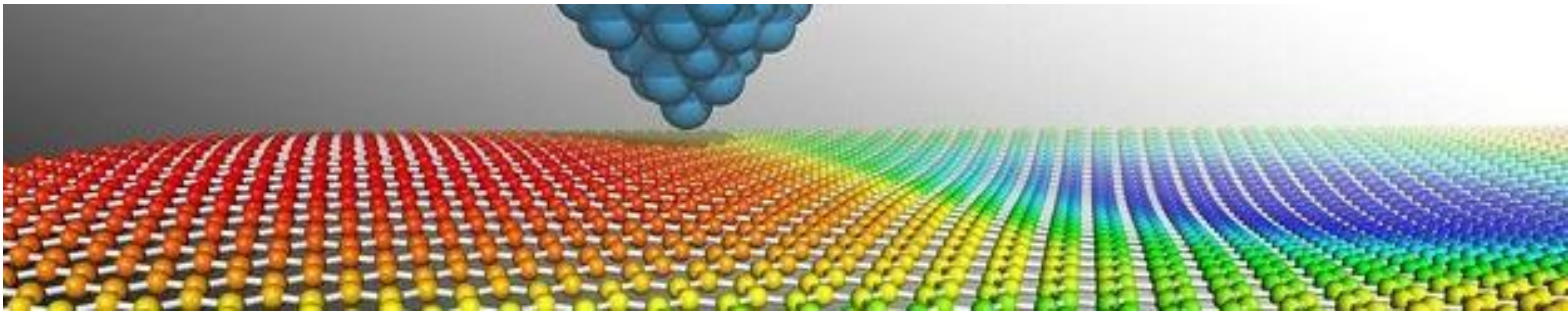

Modelling Nanostructures Symposium

A tribute to Prof. Philippe LAMBIN

University of Namur, Belgium

January 31 – February 1, 2019

UNIVERSITÉ DE NAMUR

THE SCIENTIFIC & ORGANIZING COMMITTEE

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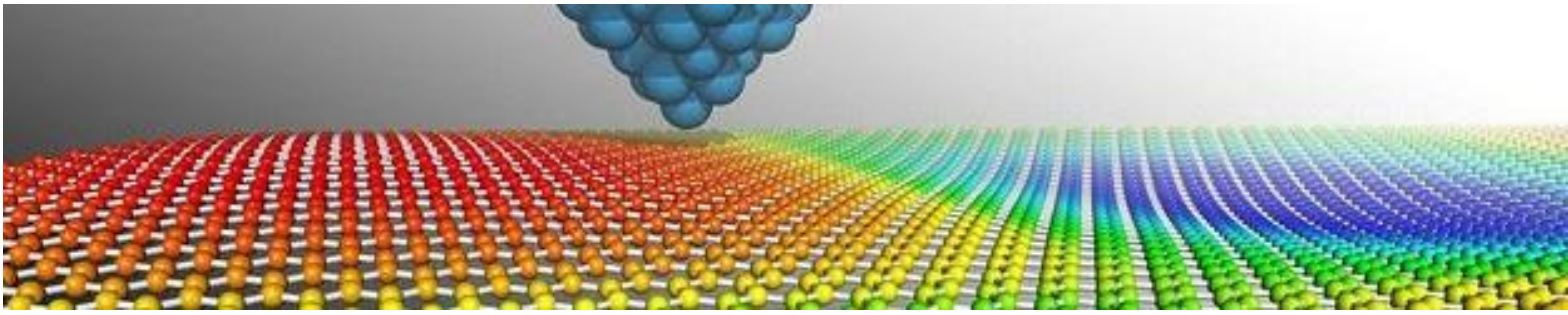


INTRODUCTION

The Symposium "Modelling Nanostructures" is organized to celebrate and honor Professor Philippe Lambin, in recognition of the many contributions he made to the field of nanoscience over the past four decades.

PROFESSOR PHILIPPE LAMBIN - AN OUTSTANDING SCIENTIFIC CAREER

As a young soon-to-be retiree from the University of Namur, and in addition to his many commitments in the service of the university and the scientific community, Philippe has had tremendous influence on a number of researchers thanks to his patient teaching, his unique approach to the training of young researchers, and his thirst to place theory/experiment collaborations at the forefront of scientific enquiry.

After completing undergraduate studies in Engineering, Philippe graduated with a PhD in Physics from the University of Liege in 1981 as a research fellow of Belgium-FNRS.

He completed a postdoctoral appointment at IBM Research Laboratory in San Jose, California before joining the University of Namur where he completed his entire career as lead researcher, for more than 35 years.

During that time, he made a number of key contributions to a field that was not yet known, at the beginning of his career, as "***nanoscience***".

The many Honors and Awards he received acknowledge his seminal and pioneering contributions to a number of scientific endeavors.

Those fields include

- Vibrational and structural properties of carbon nanotubes and graphene (theory)
- Electrodynamics of nano-structured materials
- Electronic structure of solids (tight-binding method, linear-muffin-tin orbitals)
- Propagation of elastic waves in phonic crystals
- Surface dynamics and surface electrodynamics applied to spectroscopic techniques
- Dielectric properties of multi-layered materials.

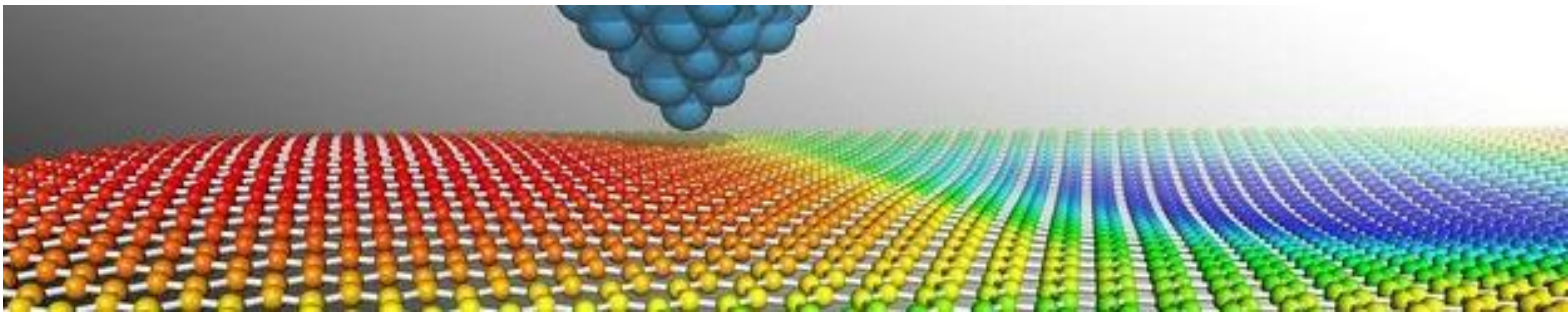
Philippe's impact on nanoscience is hard to overstate and traditional metrics (such as an h-index of 53, his 304 peer-reviewed publications, and more than 10,000 total citations) do not even start to do justice to how he shaped the current state of nanoscience research all over the world.

THE SYMPOSIUM - 31 JAN & 1 FEB 2019 - UNIVERSITY OF NAMUR

In this symposium, collaborators, former students, colleagues, and friends will gather to share their current views on the status of the field of nanoscience, and, in particular, on how theoretical modelling and computational science have enabled the understanding of nanostructured materials and the development of nanotechnology.

The focus will be on the many fields in which Philippe contributed.

It will also be an opportunity to position Philippe's influence in the greater context of current knowledge, as well as to offer a unique perspective on Philippe's legacy to science at the University of Namur and beyond.



PROGRAMME

Thursday 31 January 2019

From 9:30 | *Registration | Welcome coffee*

Morning session

Chairman: L. Henrard

10:00 | Introduction	
10:30 | Xavier Gonze	First-principles study of luminescence in phosphor materials for white-LED applications
11:10 | François Ducastelle	Excitons in hexagonal boron nitride: a tight-binding approach
11:50 | Vincent Meunier	Let's talk about phonons in low-dimensional materials
12:30 |	*Lunch | poster session*

Afternoon session – Part 1

Chairman: J-C. Charlier

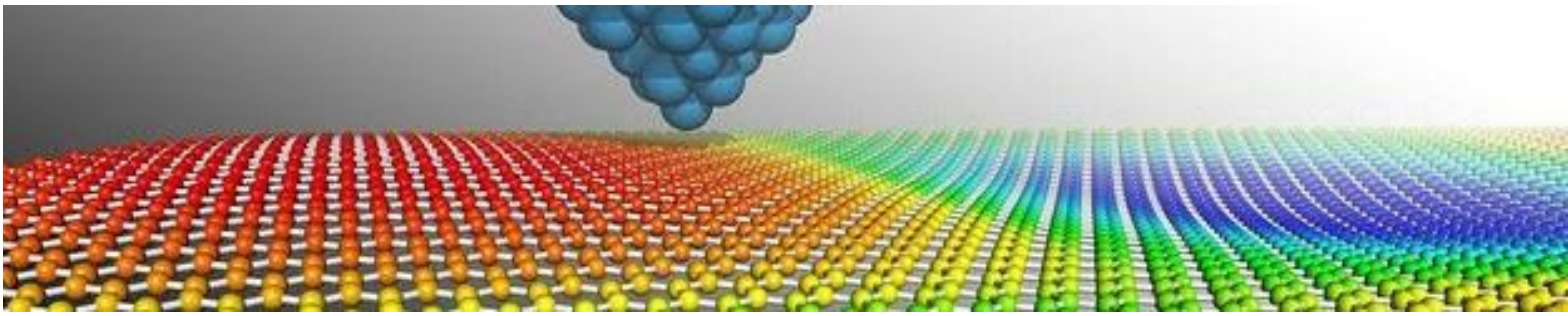
13:30 | Valentin Popov	Theoretical two-phonon Raman spectra of graphene and carbon nanotubes
14:10 | Jean-Louis Sauvajol	An experimental model system for studying coupling at the nanoscale : The individual double-walled carbon nanotubes
14:50 | Annick Loiseau	Elucidating the carbon single wall nanotube formation: where we are 25 years after their discovery
15:30 |	*Coffee break*

Afternoon session – Part 2

Chairman: R. Sporken

16:00 | Serguei Maksimenko	Propagation and generation of electromagnetic waves in carbon nanostructures
16:40 | Matthieu Verstraete	Electron beams and 2d materials
17:20 | Olivier Deparis	Modelling the scattering of light by isolated arbitrary nanostructures : the super-cell approach

18:00 \| Cheese & beer party \| poster session



PROGRAMME - Friday 1 February 2019

Morning session – Part 1
Chairman: J-F. Colomer

08:30 | Chris Van Haesendonck	Scanning probe microscopy of nanostructured materials
09:10 | Polina Kuzhir	Graphene and Carbon based metasurfaces and 3D architectures for THz applications
09:50 | François Peeters	Atomic collapse and flat bands in graphene
10:30 |	*Coffee break*

Morning session – Part 2
Chairman: V. Liégeois

11:00 | Lazslo Biro	Two decades of collaboration: from carbon nanotubes through butterflies to graphene
11:40 | Michel Devel	Modeling the electro-mechanical response of nanostructures thanks to the Gaussian QP model
12:20 | Sylvain Latil	Origami of honeycomb networks: using supercells in hexagonal lattices
13:00 |	Lunch | poster session

Afternoon session – Part 1
Chairman: J-M. André

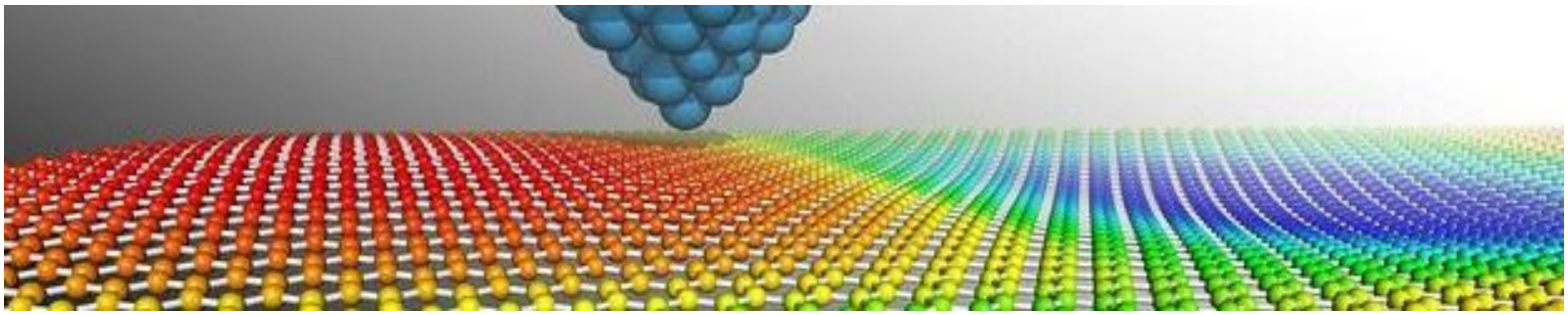
14:00 | Giorgio Benedek	Fishing for Bosons in the Fermi Sea: the He-atom Scattering Quantum Sonar
14:40 | Johan Yans	Towards a pluri/inter/transdisciplinary new and sustainable life
15:20 | Philippe Lambin	A love story...
16:00 |	*Coffee break*

Afternoon session – Part 2
Chairman: A. Lucas

16:30 |	**Tribute to Philippe Lambin**

Celebration

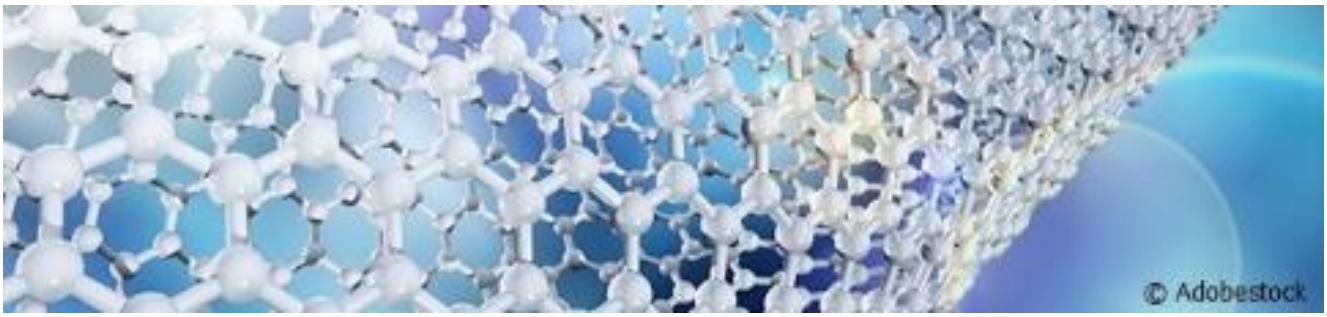
18:00 |	**Cocktail**
19:00 |	**Gala dinner**



LIST OF POSTERS

#	First name	Last Name	Poster title
1	Sofie	CAMBRÉ	DIAMETER-DEPENDENT OPTICAL ABSORPTION AND ENERGY TRANFER FROM ENCAPSULATED DYE MOLECULES TO SINGLE WALL CARBON NANOTUBES
2	Yves	CAUDANO	VIBRATIONAL SUM-FREQUENCY GENERATION (SFG) EXALTATION AT METALLIC INTERFACES. THE CASES OF DOUBLY RESONANT SFG IN FULLERENE MONOLAYERS AND OF PLASMON-ENHANCED SFG ON METALLIC NANOPILLARS
3	Evgeni	IVANOV	METHOD FOR PRODUCTION OF PLA-BASED MULTI-FUNCTIONAL NANOCOMPOSITES WITH IMPROVED PROPERTIES FOR 3D PRINTING APPLICATIONS
4	MüLLER	JÉRÔME	MULTI-SCALE MODELLING OF TCO COATING DEPOSITED BY REACTIVE MAGNETRON SPUTTERING: APPLICATION TO STRUCTURED C-SI THIN FILM SOLAR CELLS
5	Dmitry	LEVSHOV	ELECTRONIC RAMAN SCATTERING IN INDIVIDUAL DOUBLE-WALLED CARBON NANOTUBES
6	Aurélien	LHERBIER	MASSLESS FERMIONS IN 3D CARBON STRUCTURES : the missing Dirac cone
7	Marie	LOBET	CONTROLLED FLUORESCENCE IN THE PHOTONIC STRUCTURE OF EUPHOLIUS LINNEI WEEVIL'S SCALES
8	Bruno	MAJÉRUS	ELECTROMAGNETIC PROPERTIES OF MONO- AND MULTILAYERED 2D MATERIALS: APPLICATION TO GRAPHENE
9	Geza I.	MARK	WAVE PACKET DYNAMICAL SIMULATION OF DEFECTS IN 2D MATERIALS: THE HUYGENS PRINCIPLE AND THE BAND STRUCTURE
10	Alexandre	MAYER	A CHARGE-DIPOLE MODEL TO COMPUTE THE POLARIZATION PROPERTIES OF CARBON NANOTUBES AND FULLERENES
11	Sébastien	MOUCHET	NON-LINEAR AND LINEAR OPTICAL PROPERTIES OF A BEETLE'S FLUORESCENT PHOTONIC NANOSTRUCTURES
12	Mac	MUGUMAODERHA	KIVU'S COLTAN: A FACILITY FOR CHEMICAL-PHYSICS TREATMENT AND APPLICATION STUDY
13	Viet-Hung	NGUYEN	KLEIN TUNNELING AND ELECTRON OPTICS IN DIRAC-WEYL SYSTEMS WITH TILTED ENERGY DISPERSION
14	Matthieu	PAILLET	RAMAN SPECTROSCOPY OF DOUBLE-WALLED CARBON NANOTUBES
15	Mathilde	REMY	ROBUSTNESS OF ENTANGLEMENT TRANSMISSION WITHOUT PLASMONIC RESONANCE
16	Benoît	VAN TROEYE	FIRST-PRINCIPLES INVESTIGATION OF 2D LATTICE COHERENCY IN VAN DER WAALS HETEROSTRUCTURES
17	Peter	VANCSO	DEFECTS RELATED PROPERTIES IN TWO-DIMENSIONAL MOS2
18	Wim	WENSELEERS	SINGLE FILES OF DIPOLES ALIGNED IN CARBON NANOTUBES: BUILDING BLOCKS WITH GIANT NONLINEAR OPTICAL RESPONSE
19	Nils	WITTMEIER	ELECTRONIC AND TRANSPORT PROPERTIES OF SINGLE AND DOUBLE WALL CARBON NANOTUBES

Abstracts for TALKS



FIRST-PRINCIPLES STUDY OF LUMINESCENCE IN PHOSPHOR MATERIALS FOR WHITE-LED APPLICATIONS

X. Gonze[(1)], Yongchao Jia[(1)], A. Miglio[(1)], S. Poncé[(2)] and M. Mikami[(3)]

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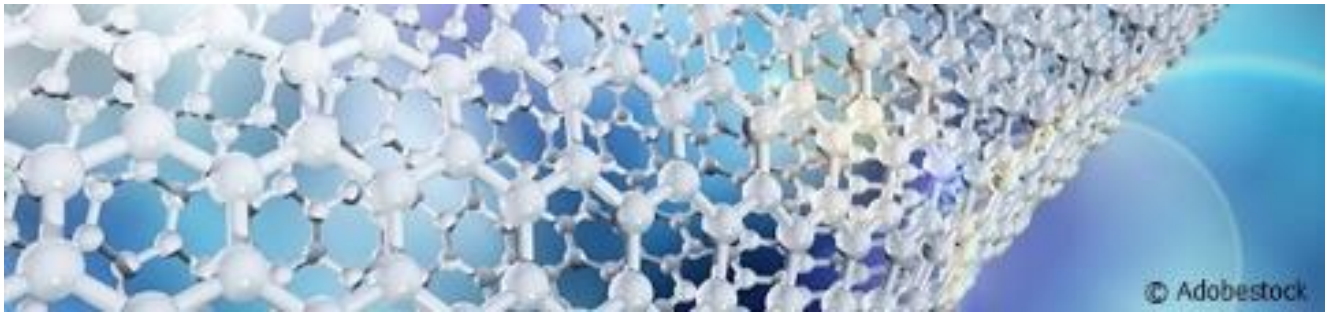
(2) Department of Materials, U. of Oxford, Oxford, UK

(3) Yokohama R&D center, Mitsubishi Chemical Corp., Yokohama, Japan

After the invasion of compact fluorescent lamps, white LED lighting is now a major contender in ecofriendly light sources, with a combination of yellow-, green- and/or red-emitting phosphors partly absorbing the blue light emitted by an InGaN LED. Phosphors with optimized luminescence properties (i.e., with an optical spectrum close to the solar one and low thermal quenching) are coveted by industry and the subject of very active development. Indeed, available blue-to-red phosphors exhibit a too wide emission linewidth or some other drawbacks, such as strong thermal quenching behavior. A detailed theoretical understanding of their combined electronic and vibronic structure is still lacking and might aid experimental researchers in finding more efficient phosphors. In view of large-scale high-throughput search for better phosphors, an accurate but fast computational methodology is needed, not restricted to the ground state (formation energy), but covering excitation and emission energies, Stokes shift, emission linewidth, and emission intensity reduction through thermal quenching.

I will first introduce the working principles of LED+Phosphor devices, the current related challenges, and the semi-empirical Dorenbos model for 4f → 5d transition energies of rare earth ions. I will then present a first-principle study of two dozen compounds, pristine as well as doped with Ce3+ or Eu2+ ions, in view of explaining their different emission color. The neutral excitation of the ions is simulated through a constrained density functional theory method coupled with a delta SCF analysis of total energies, yielding absorption energies. It matches experimental data within 0.3 eV for both absorption and emission energies (ranging between 2.0 eV and 5.0 eV) and provides Stokes shifts usually within 30%. By contrast, Dorenbos approach does not perform as well, although it provides physical insights to explain trends among the materials, including the different Stokes shifts. The first-principles approach also delivers emission linewidth and assessment of mechanisms for thermal quenching, based on a simple 1-dimensional configuration coordinate approach. For our representative set of Eu-doped materials, it is found that the 4f-5d crossover model cannot be the dominant thermal quenching mechanism: the predicted barrier at the 4f-5d crossing is always higher than 1.5 eV. In addition, it will be shown how to waive the 1-dimensional restriction in the search for the lowest 4f-5d crossing energy barrier.



EXCITONS IN HEXAGONAL BORON NITRIDE
A tight-binding approach

T. Galvani,[(2)] F. Paleari,[(2)] A. Molina-Sánchez,[(2)(3)]

L. Wirtz,[(2)] S. Latil,[(4)] L. Sponza,[(1)] H. Amara,[(1)] and F. Ducastelle[(1)]

(1) Laboratoire d'Etude des Microstructures, ONERA-CNRS, BP 72, 92322 Châtillon Cedex, France

(2) Physics and Materials Science Research Unit, University of Luxembourg,

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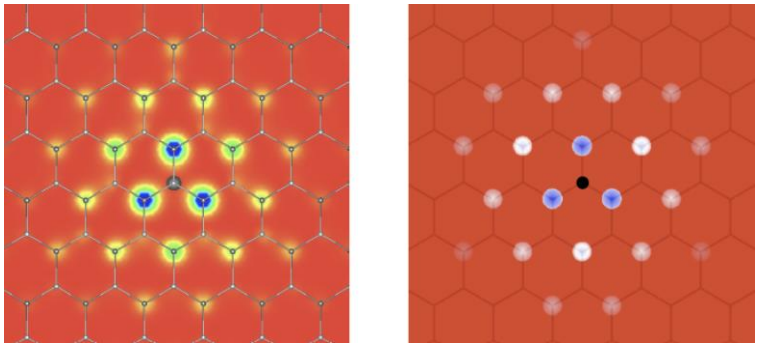
(4) SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay 91191 Gif sur Yvette, France

After the exceptional interest attracted by graphene, numerous studies have been devoted to 2D materials and to those lamellar compounds which can be easily exfoliated. After MoS_2, semiconducting transition metal chalcogenides have been the object of increasing researches, in particular after the discovery of their interesting optical properties. Hexagonal boron nitride on the other hand is very similar to graphene and has a very large gap, about 6 eV, and is a an insulator which has interesting properties in the engineering of epitaxial van der Waals heterostructures.

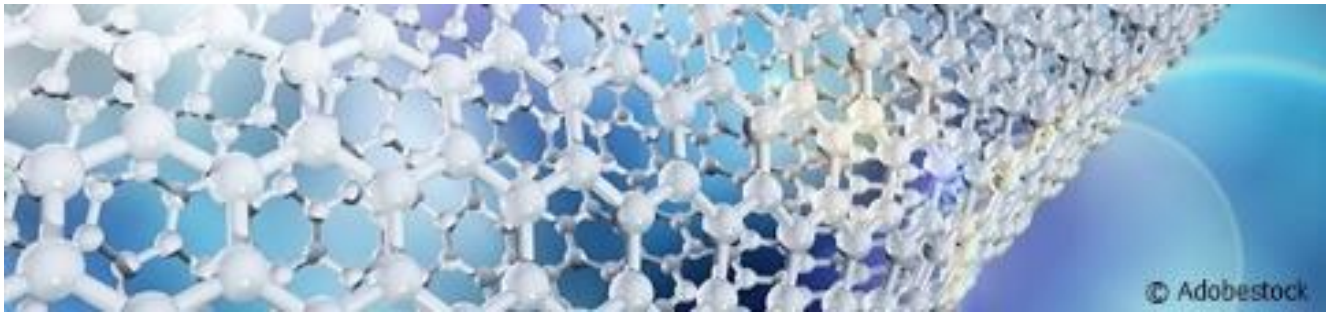
Its optical propeties, in the far UV range are difficult to study experimentally, but potentially very interesting too. Because of its very simple electronic structure hBN is a very good system to develop and test theoretical models to understand the particular excitonic properties of 2D materials. Contray to usual 3D semiconductors, excitons play here a very important part, but the usual hydrogenic models to describe Wannier-Mott excitons are not really adapted.

We will present here a very simple model to understand the excitonic properties of hBN based on a simple tight-binding description of the π electronic states. It is in excellent agreement with ab initio calculations based on the Bethe Salpeter equations[1] and allows us to treat different problems : non-linear optical properties[2] as well as the competition between direct and indirect excitons.[3]



hBN single layer: Total probability electronic density of the ground- state degenerate exciton states when the hole is located just above a nitrogen atom. Left: ab initio calculation; right: tight-binding calculation.[1]

1. T. Galvani et al. Phys. Rev. B 94, 125303 (2016)
2. C. Attaccalite et al. Phys. Rev B 98, 165126 (2018)
3. L. Sponza et al. Phys. Rev 98, 125206 (2018)



LET'S TALK ABOUT PHONONS IN LOW DIMENSIONAL MATERIALS

V. Meunier

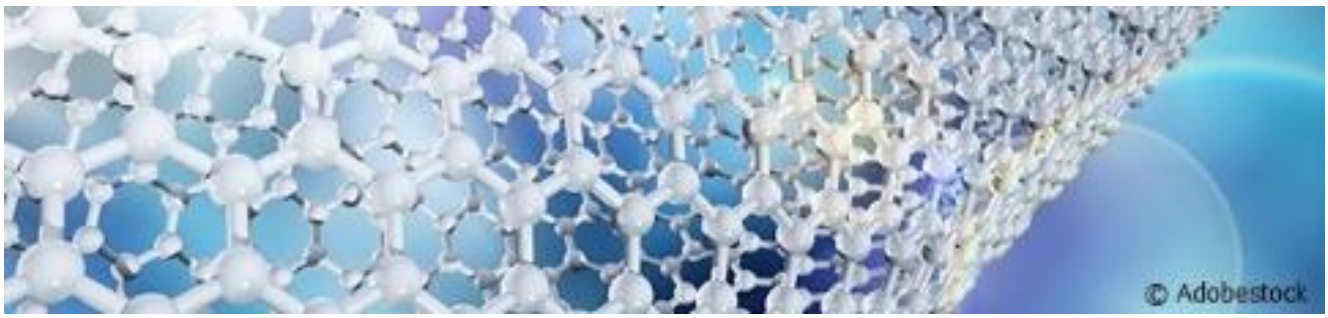
Rensselaer Polytechnic Institute

2D materials (2DMs) such as graphene, transition metal dichalcogenides (TMDs) and black phosphorus have attracted significant attention as emerging low-dimensional materials. These materials feature an array of properties that offer many promises in terms of potential electronic and optoelectronic applications.

Many characterization techniques have been employed to improve the understanding of these materials, to establish their crystal structure, purity, number of layers, and internal arrangements. In particular, Raman spectroscopy, has demonstrated that structural vibrations can be used as solid indicators of the structural properties of 2DMs.

However, due to the emergence of new properties, the interpretation of experimental features requires a dedicated modeling effort based on quantum-mechanics.

In this talk, I will overview how quantum mechanical properties and non- resonant Raman scattering are combined to determine the fundamental structural properties in a broad array of 2D materials. I will discuss the importance of low-frequency modes in the study of layer-layer interactions in 2DMs, and how relative twisting angles between layers can be determined by monitoring relative shifts in Raman active mode. I will also show how vibrational signatures can be exploited to understand in-plane anisotropy in phosphorene.



THEORETICAL TWO-PHONON RAMAN SPECTRA OF GRAPHENE AND CARBON NANOTBES

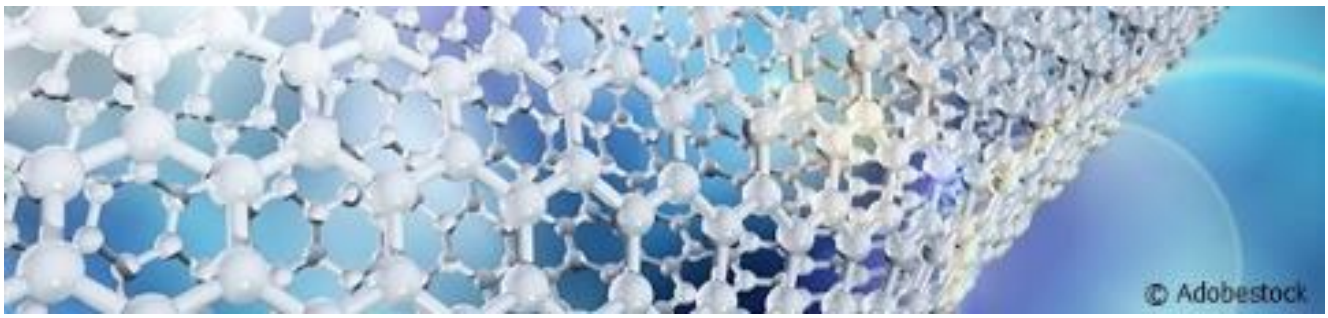
V. N. Popov[(1)] and Ph. Lambin[(2)]

(1) Faculty of Physics, University of Sofia, BG-1164 Sofia, Bulgaria

(2) Département de Physique, Université de Namur, B-5000 Namur, Belgium

We review the recent progress in the calculation of the two-phonon Raman bands of graphene and carbon nanotubes. We compare our results, derived within the non-orthogonal tight-binding model, with available theoretical and experimental data. We show that the tight-binding approach allows to effectively grasp the main features of the experimental two-phonon Raman bands.

Acknowledgements: This work was supported by the National Science Fund of Bulgaria under Grant No. DN18/9-11.12.2017.



DOUBLE-WALLED CARBON NANOTUBES

A unique model system for studying coupling at the nanoscale

M. Paillet[(1)], D. Levshov[(1)], T. Michel[(1)], H. N. Tran[(1)], R. Parret[(1)], A. A. Zahab[(1)] and J.-L. Sauvajol[(1)]

(1) Laboratoire Charles Coulomb (L2C), Université de Montpellier, Montpellier, France

Using an experimental approach that combines high-resolution electron microscopy, electron diffraction and optical spectroscopies, including Raman scattering, Rayleigh spectroscopy and photoluminescence, on individual, spatially isolated and suspended (free-standing) single-walled (SWNTs) and double-walled carbon nanotubes (DWNTs), we have been able to investigate their phonons characteristics and optical properties.

In this talk, we present an overview of the most significant results obtained via this approach. Particular attention is paid to the study of DWNTs, a coaxial composite of two SWNTs, which provide a unique model system for studying coupling at the nanoscale. We show how such coupling, originating from the van der Waals interaction between the inner and outer nanotubes, plays a crucial role in determining the characteristics of the collective radial breathing-like modes and G modes in DWNTs (for a review see Ref. 1-2). The effects of quantum interference between different electronic transitions on the experimental behavior of the G-modes intensity are discussed [3].

It must be emphasized that the theoretical predictions of Philippe Lambin and his collaborators have been invaluable in understanding a lot of these experimental data [4].

References:

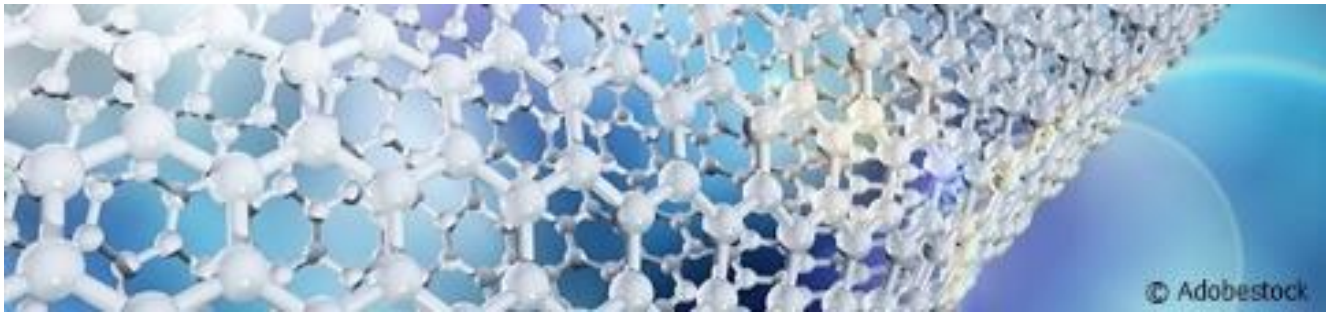
1. T. Michel et al. in "Optical properties of carbon nanotubes: a volume dedicated to the memory of Mildred Dresselhaus", Handbook of Carbon Nanomaterials, Vol. 10, ISBN: 978-981-3235-45-8 (2019) and references therein.

*2 .D. Levshov et al. , Carbon **114**, 141 (2017) and references therein.*

*3. H. N. Tran et al. Phys. Rev. B **95**, 205411 (2017)*

*4. V. Popov and P. Lambin Phys. Rev. B **73** 085407 (2006); Phys. Rev. B **73**, 165425 (2006); Nano Res. **11** 822 (2010)*

Acknowledgements:
We thank Philippe Lambin, Luc Henrard, Valentin Popov and Jean-Roch Huntzinger for helpful discussions during all these last years. We thank Raul Arenal for the electronic microscopy studies conducted at the "Laboratorio de Microscopías Avanzadas" at the Universidad de Zaragoza, (Spain) and Thi Thanh Cao, Van Chuc Nguyen and Ngoc Minh Phan for the synthesis of carbon nanotubes made at the "Institute of Materials Science of the Vietnam Academy of Science and Technology" in Hanoi (Vietnam).



ELUCIDATING CARBON SINGLE WALL NANOTUBE FORMATION: Where we are 25 years after their discovery?

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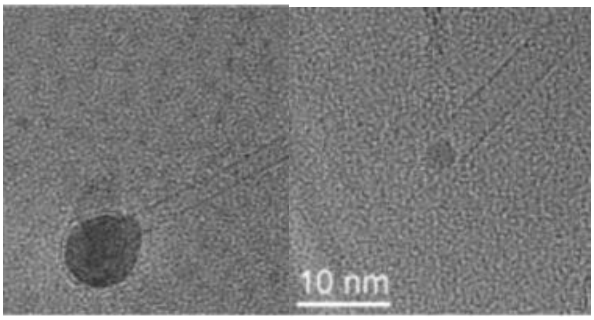
(1) Laboratoire d'Etude des Microstructures, CNRS-ONERA, University Paris Saclay, Chatillon, France

(2) Aix Marseille Université, CNRS, Centre Interdisciplinaire de Nanoscience de Marseille, Marseille, France

Carbon multi wall nanotubes (MWNTs) and single wall nanotubes (SWNT) have been identified by S. Ijima in 1991 and 1993 respectively. Although significant progress has been made since 25 years, one major obstacle to realization of SWNTs-based nanotechnology has been the lack of control for designing selective synthesis conditions. This is partly due to the incomplete understanding of the physical and chemical effects driving the kind of tubes able to nucleate and grow under given experimental conditions [1].

It is now well established that SWNTs formation mechanism is based on a dissolution – segregation process of carbon at the surface of the metallic nanoparticles [2]. Therefore controlling the state of the particles and their link with the growing tubes is essential for controlling the structure of the tubes. In this context, an enlightening approach is to perform systematic *ex situ* TEM studies of the SWNTs and to inspect their structure, their link with the metal particles and the nanoparticle structure in a statistical way [2, 3]. Thanks to this approach, we have identified two nucleation and growth modes, so- called 'tangential' and
'perpendicular', corresponding to different nanotube-particle junctions [3]. With the support of atomistic simulations [3, 4], we have established and verified with designed specific growth experiments that the growth mode is directly linked with the carbon content of the nanoparticle [5].

A second fruitful approach is to consider SWNT growth from a thermodynamic point of view. To that aim, we have developed a statistical thermodynamics model, which relates the stable tube structures to the tube/catalyst interfacial energies for zigzag and armchair edges and to the temperature [6]. The efficiency of this model will be shown for understanding the origin of the frequently reported near-armchair selectivity in perpendicular growth mode [5] and for accounting for observed chirality distributions under given synthesis conditions. Finally the potential of the model will be evaluated for providing guidelines for catalyst design and growth condition optimization.



HRTEM images of SWNT grown according to the perpendicular mode (left) and the tangential mode (right)

References

*1. Amara H. and C. Bichara C., Topics in Current Chemistry **375**, 55 (2017)*

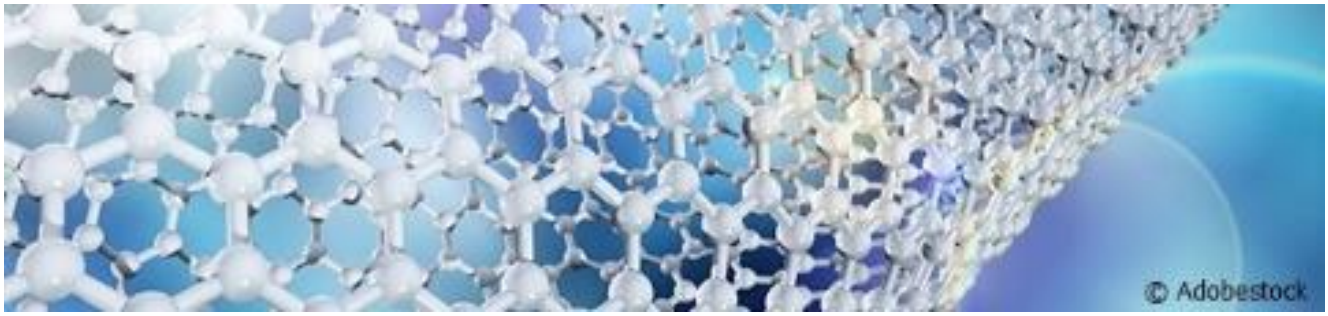
*2. J. Gavillet et al, Phys. Rev. Lett. (2001), **87**, 275504*

*3. M.-F. C. Fiawoo et al., Phys. Rev. Lett. (2012).**108**, 195503*

*4. M. Diarra et al., Phys. Rev. Lett. (2012), **109**, 185501*

*5. He, M. et al. Nanoscale (2018), **10**, 6744-6750*

*6. Magnin, Y. et al, Science (2018) **362**, 212-215*



PROPAGATION AND GENERATION OF ELECTROMAGNETIC WAVES IN CARBON NANOSTRUCTURES

K. Batrakov(1), S. Maksimenko(1) and M. Shuba(1)

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Propagation and generation of electromagnetic waves in graphene and carbon nanotubes (CNTs) is considered. Electromagnetic scattering theory is applied to calculate polarizabilities of finite-length single- and multi -walled carbon nanotubes (SW- and MWCNTs) in terahertz and IR ranges. It is shown that electromagnetic response of graphene and carbon nanotubes is characterised by a strong slowing down of surface waves (plasmon-polaritons) propagating over such structures [1,2]. Antenna properties of CNTs and CNT bundles are described. We demonstrate theoretically the dominant role of finite size effect in the non-Drude conductivity of CNT films due to the strong slowing down [3]. The experimental evidence of the CNT length dependence of the THz spectra of SWCNT films [4] is presented. We demonstrate that surface plasmon-polariton waves with low phase velocity in carbon nanostructures can be utilized for the generation of coherent terahertz radiation through the Cherenkov mechanism, the effect being expected to be observable in carbon nanotubes and being especially pronounced in spatially expanded double- and multi-layer graphene structures owing to the suppression of the inter-layer tunnelling [5-7]. In addition to a strong slowing down, other two basic properties of graphene and carbon nanotubes, anomalously large electron free pass length, and extremely high electron current density reachable in structures, are considered, allowing proposing them as candidates for the development of nanoscale Cherenkov-type emitters, analogous to traveling-wave tube and free electron laser. In graphene/polymer multi-layered structures exposed to external electron beam, the generation is possible on macroscopic scale, and generation frequency tuning appears to be possible by varying the graphene doping, the number of graphene sheets, the distance between sheets, etc. Theoretical and experimental results on absorption in and reflection from graphene/polymer sandwiches are analysed as evidence of a strong electromagnetic field/graphene structure coupling [8-9].

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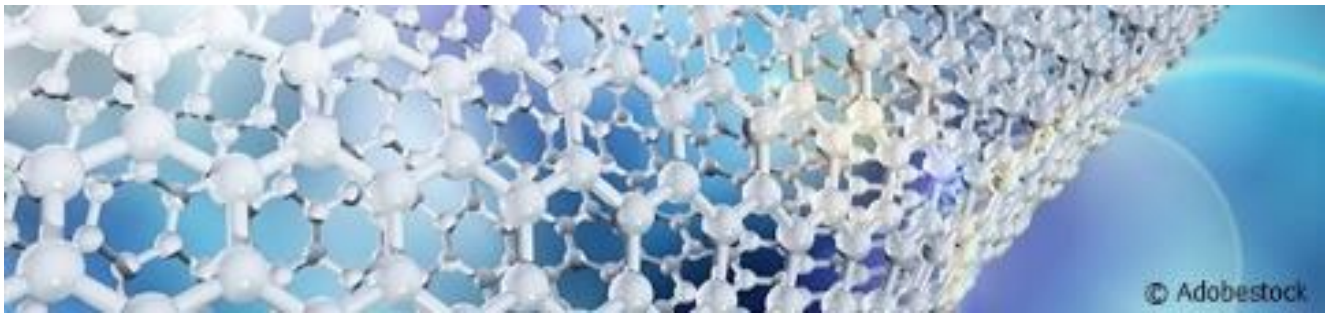
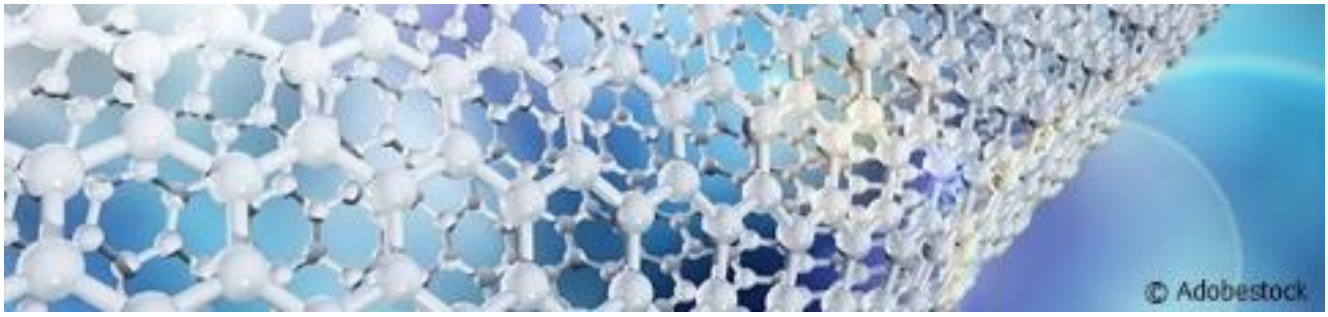


ELECTRON BEAMS AND 2D MATERIALS

M. Verstraeten

Université de Liège

Electron microscopy is the most powerful technique we have to access the nanoscale structure of matter. 2D materials are a natural target for TEM and EELS, being intrinsically thin and showing exotic physics. I discuss how to conversely use 2D materials to benchmark TEM, and how to use first principles simulations to understand and control atom-scale bits.



MODELLING THE SCATTERING OF LIGHT BY ISOLATED ARBITRARY NANOSTRUCTURES: THE SUPER-CELL APPROACH

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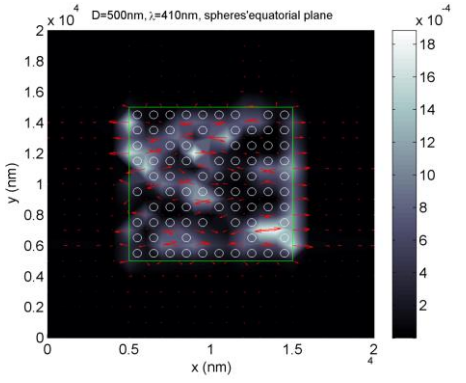
Scattering of light by isolated arbitrary nanostructures is not only of fundamental interest but has also many applications. For instance, planar solar concentrators may be conceived, in which radiation normally incident to the slab is partly redirected towards its lateral faces thanks to scattering by embedded nanostructures such as a collection of dielectric spheres (see Figure). Evaluating the lateral energy flux requires to calculate the Poynting vector locally. In infinite periodic media (photonic crystals), an exact expression of the local Poynting vector can be obtained analytically [1]. In arbitrary inhomogeneous media, on the other hand, it must be computed numerically. As far as scattering of light by an isolated arbitrary structure is concerned, the time-domain finite difference (FDTD) method, introduced by Yee in 1966, is probably an obvious choice for modelling. However, numerical simulations can be highly time-consuming since time-dependent electric and magnetic fields must be calculated at every point of a 3D spatial grid (Yee's cell) whose spacing is imposed by the nanostructure's size and morphology. Moreover, the need to suppress non-physical reflections of the scattered wave on the computing box boundary surfaces requires using perfectly matched layers (Berenger, 1994) whose numerical implementation is far from being straightforward. On the other hand, the rigorous coupled wave analysis (RCWA) method, which was developed in the 80'ies for modelling periodic corrugations (gratings), could be an alternative choice, would not be the lateral periodicity requirement imposed on the structure. At first glance, it seems illusory to call RCWA for modelling an isolated structure, since the method requires repeating the arbitrary structure (defined in the unit cell) infinitely in lateral directions (Bloch boundary conditions). Fortunately, the super-cell concept, which is well known in modelling of electronic structures, allows us to circumvent this problem. Actually, we already applied it to model light trapping in solar cells by random nanocorrugations [2]. The idea is that the structure within the unit cell can be arbitrary defined, for instance as disordered arrangement of scattering objects. If the super-cell is sufficiently large compared to structure's details, then the periodicity introduced by Bloch conditions at the cell's boundary can be regarded as purely artificial, producing a quasi-disordered structure with infinite lateral size [2]. This concept is exploited here for a different purpose: i.e. modelling an isolated arbitrary structure instead of an infinite quasi-disordered structure. Therefore, care must be taken so that the mirrored structures in adjacent super-cells do not couple to each other. In theory, it is impossible. In practice, it can be achieved by foreseeing a sufficiently large distance (guard) between the structure and the super-cell boundary. In this talk, I shall present preliminary RCWA simulation results on the scattering of light by isolated nanostructures and I shall discuss about pros and cons of using a super-cell approach for modelling.



Poytning vector (in-plane projection) and map of its normalized out-of-plane projection calculated by RCWA using super-cell approach.

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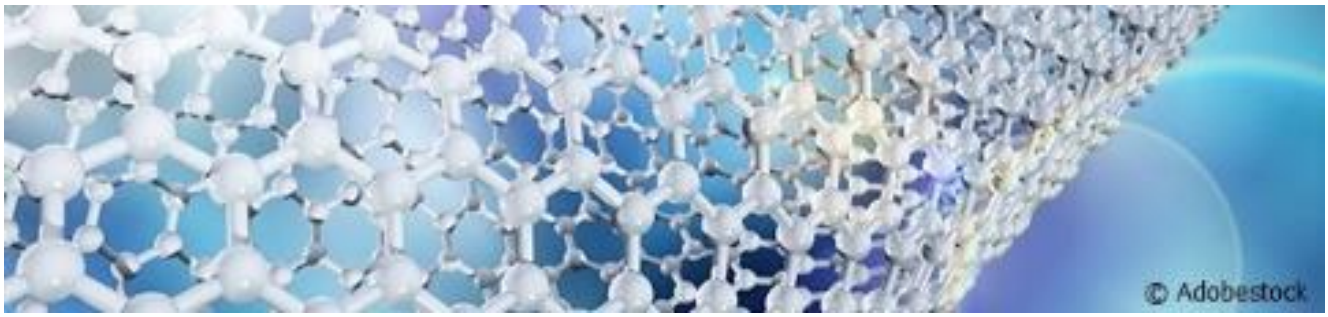

SCANNING PROBE MICROSCOPY OF NANOSTRUCTURED MATERIALS

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Scanning probe microscopy (SPM) has emerged as a powerful tool for characterizing and manipulating surfaces down to the atomic scale. I will illustrate the unique possibilities provided by SPM to investigate the functional properties of nanostructured surfaces and to link these properties to the surface structure. Two of the most often used SPM variants, i.e. scanning tunneling microscopy (STM) and scanning force microscopy (SFM), will be considered.

After giving an overview of the different functionalities that can be probed, I will focus on our studies of carbon nanotubes and of graphene using STM and SFM. These studies include in particular the electronic, mechanical and electromechanical properties of straight and coiled nanotubes, and the electronic and mechanical properties of graphene. The figures below present two typical results.

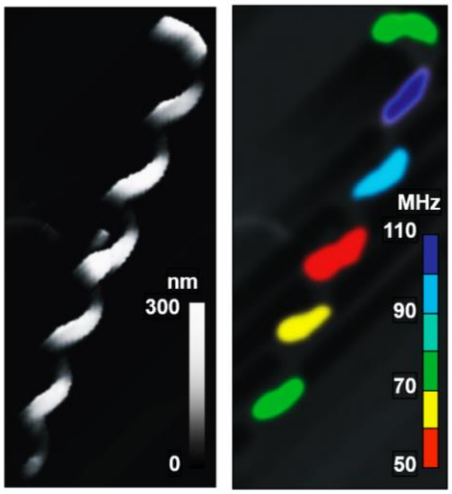

Fig. 1. SFM of a coiled multiwalled nanotube deposited on an oxidized silicon wafer. The left image is a topographic image. The right image shows the mechanical resonances of the nanotube windings that are detected by the tip of the SFM when exciting substrate oscillations at different frequencies.

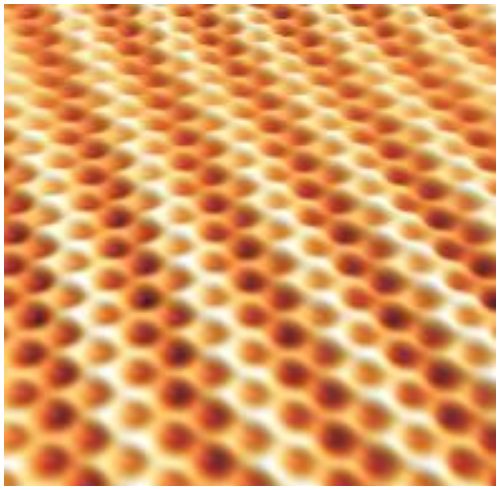

Fig. 2. Three-dimensional Fourier-filtered STM image of graphene that has been grown on Al_2O_3(0001)/Cu(111) using chemical vapor deposition. The alternating bright/dark stripe-like structure can be linked to the presence of a Moiré pattern[1].

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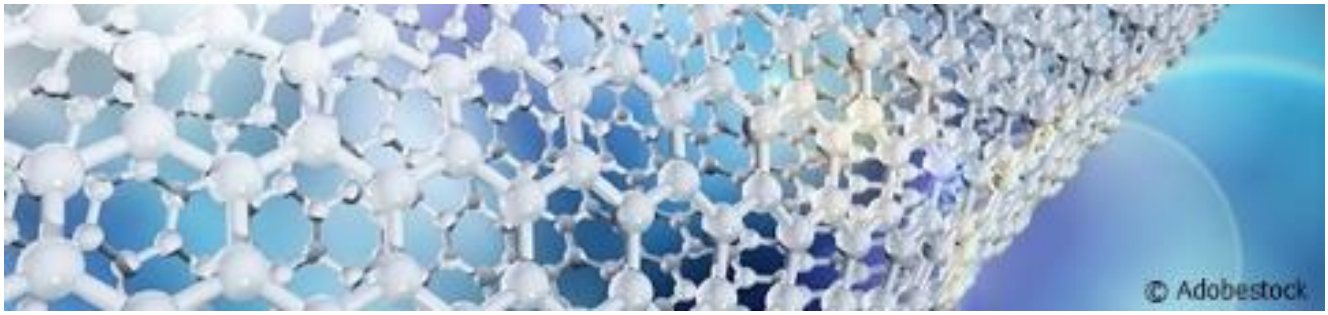

GRAPHENE AND CARBON BASED METASURFACES AND 3D ARCHITECTURES FOR THZ APPLICATIONS

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The problems of periodic concentration of electromagnetic (EM) field as well as perfect absorption of THz radiation are among the hottest issues of electromagnetics now. This is because these effects underline a physical background for many of technological breakthroughs, such as ultra-sensitive detectors of electromagnetic pulses, compact waveguides and collimators, and even unconventional EM memory.

Carbon porous structures are known for many years as effective ultra-light electromagnetic shields [1]. However, being made of highly conductive carbon skeleton (the conductivity is in the range from a few thousands to a few tens of thousands S/m) they demonstrate high reflection ability of sub-microwave radiation. It has been recently shown [2] that highly conductive skeleton is responsible for the sharp resonance absorption peaks at given frequencies (in most cases in THz frequency ranges), which position corresponds to the cell and/or window size of glassy carbon-based meshes.

The abilities of regular meshes made by probably the simplest technological route, which is additive manufacture, are just mentioned in a very few publications [3]. At the same time, printable and therefore easily reproducible lossy tunable photonics crystals could solve a number of materials related problems in modern applied electromagnetics. We will present the modeling results of the EM response of 3D printed regular architectures vs their lattice parameters in view of their skeleton conductivity.

The advantages of having structures (i) made of highly conductive carbon skeleton and (ii) being produced from the carbon-containing polymer with much smaller conductivity will be analyzed. The peculiarities of EM response of thin carbon films and graphene-based metasurfaces will be also highlighted.

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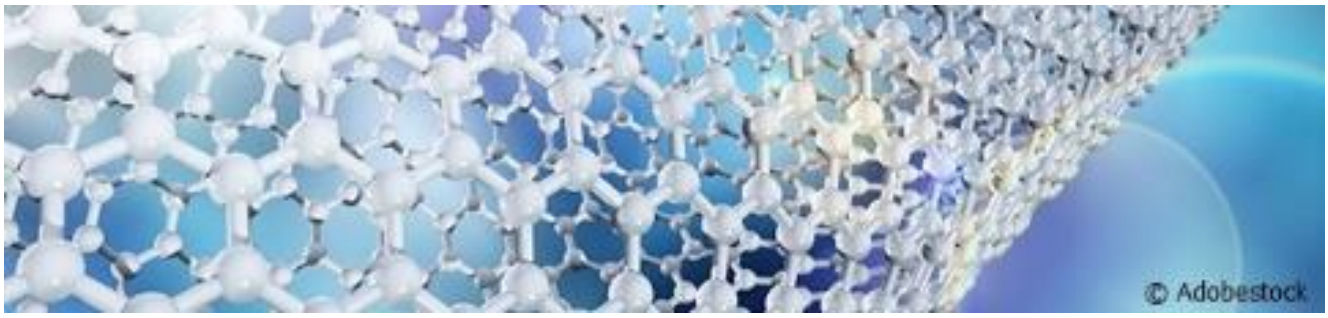

ATOMIC COLLAPSE AND FLAT BANDS IN GRAPHENE

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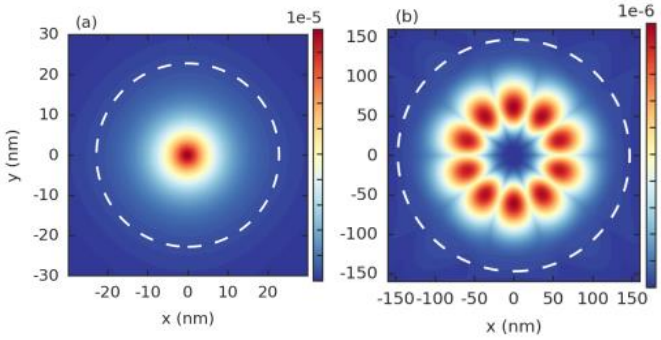
Quantum electrodynamics predicts that heavy atoms ($Z > Z_c \sim 170$) will undergo the process of *atomic collapse* where electrons sink into the positron continuum and a new family of so-called *collapsing* states emerges. This phenomenon has never been confirmed experimentally. The wonder material graphene has made it possible to investigate[1] similar physics in two dimensions using vacancies with tunable charge where the 'atomic' collapse occurs at a much lower critical charge ($Z_c \sim 1$).



The transition from sub-critical to the supercritical regime is accompanied by trapping of electrons in quasi-bound states which are the condensed matter analogue of the long sought after phenomenon of atomic collapse in super-heavy nuclei. The quasi-bound electron-states show up as a strong enhancement of the density of states within a disc centered on the vacancy site. We find that these states are surrounded by a circular halo of hole states which are interpreted as the analogue of positron production in atomic collapse. We further show that the quasi-bound states at the vacancy site are gate tunable and that the trapping mecanism can be turned on and off, providing a new paradigm to confine, control and guide electrons in graphene.

Recently[2], we found that a sharp STM tip is able to induce similar atomic collapse states (see Fig. a). For large tip potentials a sub-micrometer scale p-n junction is induced that exhibits *whisper gallery modes* (see Fig. b). Thus the STM tip allows us to tune a circular p-n junction in graphene from quantum confinement to optical guiding.

We realized[3] a periodic buckling structure of a single graphene layer. Because of the periodic strain the electrons are subject to a periodic *pseudomagnetic field* that does not break time reversal symmetry. Through a detailed STM spectrum mapping and tight binding calculations, we reveal the possibility of generating a robust flat band. This buckling method should enable us to design flat bands with different superlattice symmetry which is inaccessible by the moiré superlattices method that was recently realized for magic angle twisted bilayer graphene[4].

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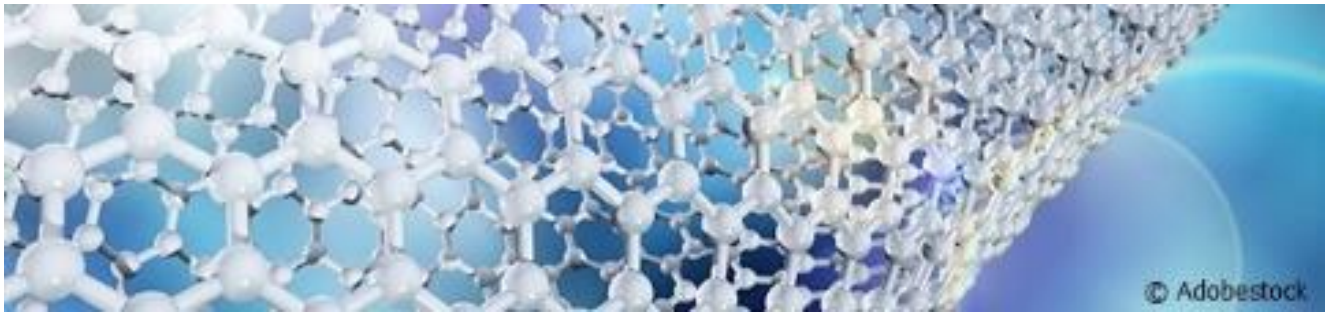

TWO DECADES OF COLLABORATION:

From carbon nanotubes through butterflies to graphene

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Our collaboration with Prof. Lambin spanned over perhaps the most exciting period of the formation of Nanoscience. We first met at the E-MRS in 1995, I was talking on the STM characterization of KC_{60} linear polymer – built like a necklace of pearls from C_{60} molecules - Prof. Lambin and Prof. B.Nagy were presenting their results on the catalytic CVD growth of the carbon nanotubes (CNT). They invited me for a to Namur for a short visit, which took in place in 1996, we showed that it is possible to grow SWCNTs by CVD [1].

In the following two decades I spent altogether 60 months in Namur with the generous funding of the FNRS. During this time, very exciting work was carried out that ranged from exotic carbon nanotubes, like the regularly coiled ones, Fig. 1 [2], through the structural colors of wonderful butterflies [3], to the characterization and atomic precision patterning of graphene, Fig. 2. [4].

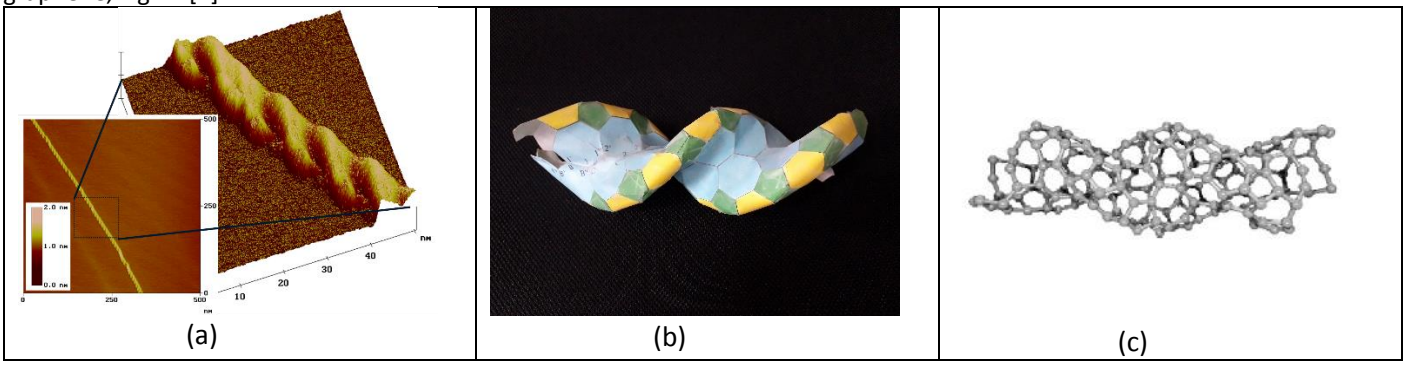

Fig. 1. Observation and modelling of coiled carbon nanotubes [2]. (a) Experimental scanning tunneling microscope image; (b) paper model; (c) relaxed computer model.

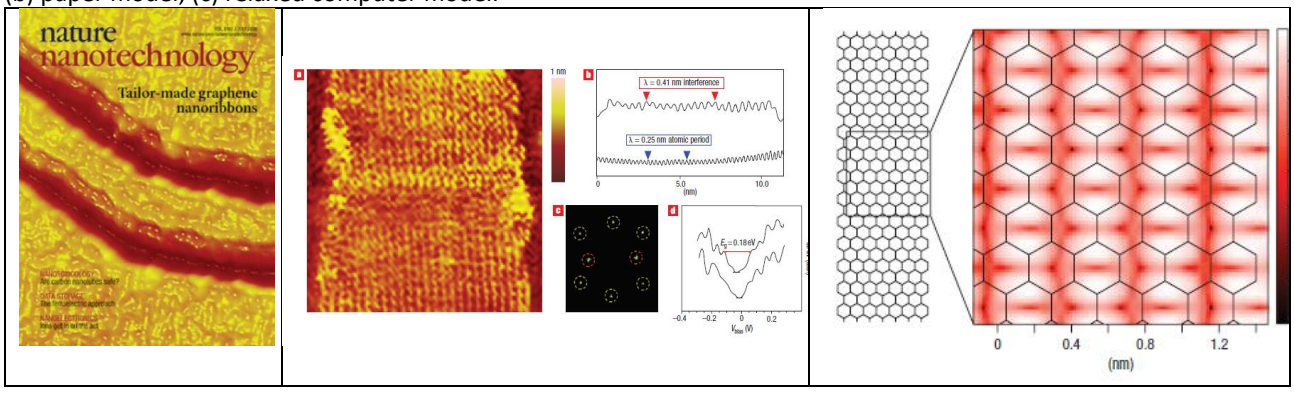

Fig.2 Armchair and zig-zag graphene nanoribbons cut by STM lithography and computed STM image [4].

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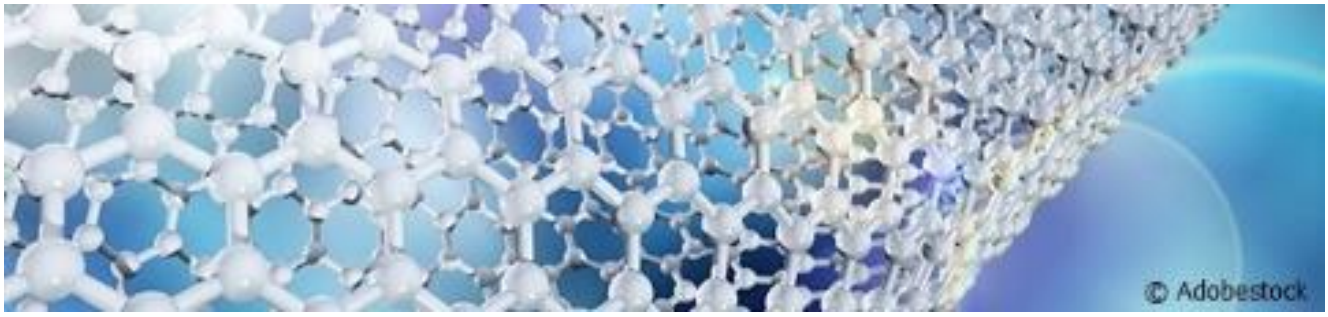

MODELLING THE ELECTRO-CHEMICAL RESPONSE OF NANOSTRUCTURES THANKS TO THE GAUSSIAN QP MODEL

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In their pioneering work introducing an atom monopole-dipole interaction model with charge transfer for the treatment of polarizabilities of π-bonded molecules, Olson and Sundberg (J. Chem. Phys., **69**, 5400 (1978)), used self-consistently determined atomic charges and dipoles to compute the response of an extended molecule to an external electric field. Soon after, it was realized by Thole (Chem. Phys., **59**, 341 (1981)), that for nearest neighbour atoms, the interaction tensors between charges and dipoles should be adapted from their vacuum value (by convolution with a regularization function, mimicking the radial distribution of charges around the nuclei) in order to remove possible spurious effects such as "polarization catastrophes".

Thanks to several exchanges between researchers from Namur and Besançon during the 1990's and 2000's, we could adapt these methods to fullerene onions, carbon nanotubes and graphene. Then, taking advantage of work started under the supervision of Ph. Lambin, we coupled these electrostatic calculations with the AIREBO potential, in order to study the mechanical bending response of carbon nanotubes to an externally applied electrostatic field[1]. However, owing to the 'large' size of carbon nanotubes and their environment in realistic nanoelectromechanical systems, we began developing some bridging technique between atomistic simulations and continuum physics allowing us to embed both mechanical and electrostatic atomistic information in a single continuum variational approach[2]. This lead to the possibility of a coupled atomistic / continuum physics approach for the computation of the flexoelectric coefficients of carbon nanotubes [3 and G. Lecoutre's PHD thesis, 2018].

Finally, if time allows, I may discuss how we have begun parameterizing the Gaussian regularized QP model for transition metal dichalcogenide 2D materials such as MoS_2[4].

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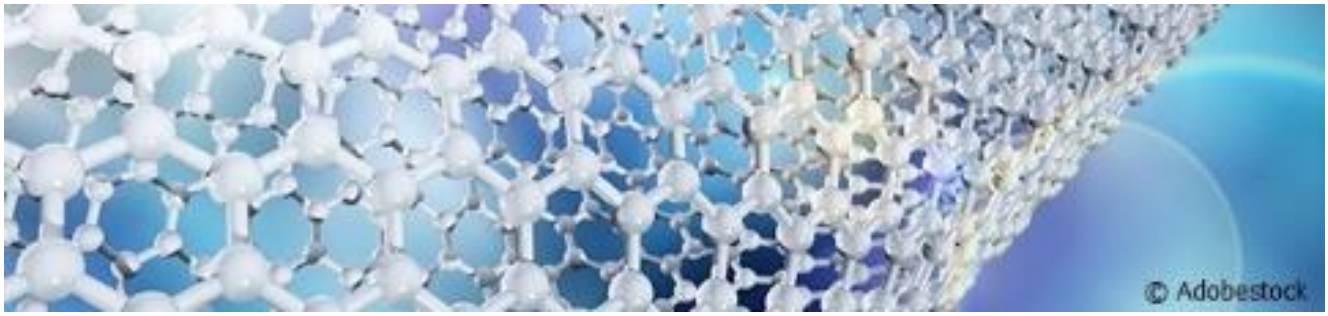

ORIGAMI OF HONEYCOMB NETWORKS:

Using supercells in hexagonal lattices

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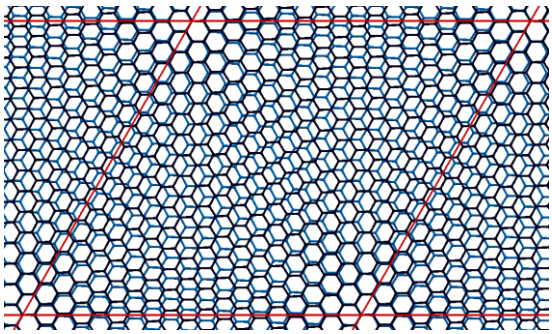
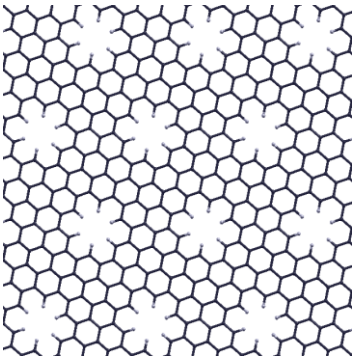
The Bloch theorem is the master tool of the solid-state theory, at the base of most electronic calculation techniques. It is not totally suitable for nano-structures, since they lie in between the crystal and isolated molecule.
However, in systems for which the translational symmetry is modified (surface reconstruction, molecular self-organization), is locally broken (point defects, edges) or does not simply exist (large clusters or molecules), the Bloch theorem can be used with the help of supercells.

After briefly introducing the concept of supercell, I will show how to recover a quasi-band structure by means of Brillouin zone unfolding [1].

I will give examples of the use of supercell for the theoretical study of carbon nanostructures electronic properties. Attention will be paid to our former *made-in-Namur* works : point defects in graphene [2] and turbostratic stacking of graphene layers [3]. Later, I will present our new project dedicated to periodically holed graphene (“anti-dot” lattices), that have been proposed a decade ago [4].





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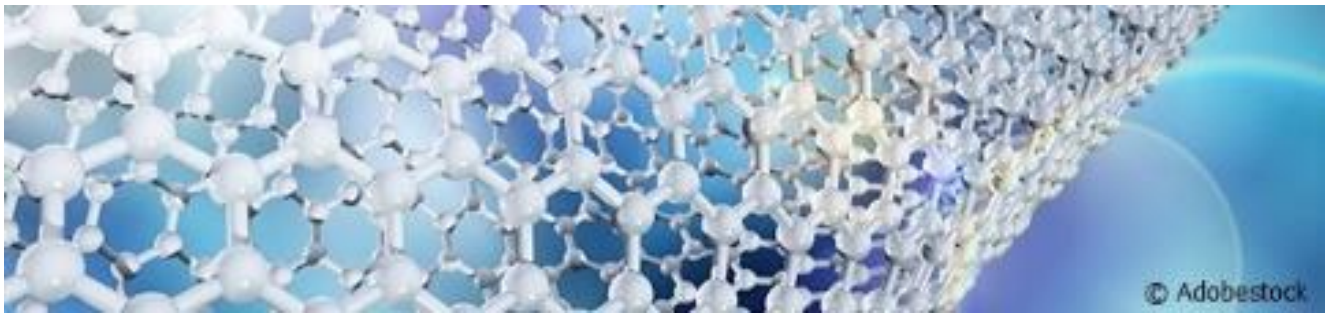

FISHING FOR BOSONS IN THE FERMI SEA

The He Atom Scattering Quantum Sonar

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The development of supersonic monocromatic (ΔE < 0.5 meV) ^{4}He-beam and of ^{3}He spin-echo (3He-SE, ΔE < 0.5 μeV) spectrometers has paved the way to high-resolution momentum- resolved spectroscopy of surface dynamics with He-atom scattering (HAS)[1]. Unlike thermal neutrons and X-rays, thermal neutral He atoms only tickle the surface ~0.3 nm away from the first atomic plane, and exchange energy and momentum with the solid atoms only via the interposed electrons. Thus phonons are detected via the electron-phonon (e-ph) interaction, and not just at the surface, but possibly as deep below the surface as the range of that interaction. This sort of *quantum sonar* allows for the direct measurement of the e-ph coupling strength for each individual phonon (*mode-λ spectroscopy*)[2,3], and for ultimately answering the question about phonon-mediated pairing in (2D-) superconductors: who's doing the job? The venerable concept of Debye-Waller (DW) factor, by which Piet Debye and Ivar Waller in 1923 correctly attributed to thermal vibrations the attenuation of Roentgen rays, in the case of HAS and 3He-SE from conducting surfaces presently allows for a direct measurement of the e-ph mass-enhancement factor λ - a basic parameter for conducting materials. In particular much can be learnt with HAS and 3He-SE about layer topological insulators (TIs)[5], their peculiar surface electronic structure and related e-ph coupling, as it will be shown with a few recent examples. Selfish surface electrons, when hit by a He atom, may however decide to keep for themselves the received energy and momentum, rather than delivering them to phonons. Thus HAS is also qualifying as a possible probe of surface electron excitations in the THz domain, such as acoustic surface plasmons, CDW phasons and Fermi-surface inter-pocket transitions in semimetal topological insulators.

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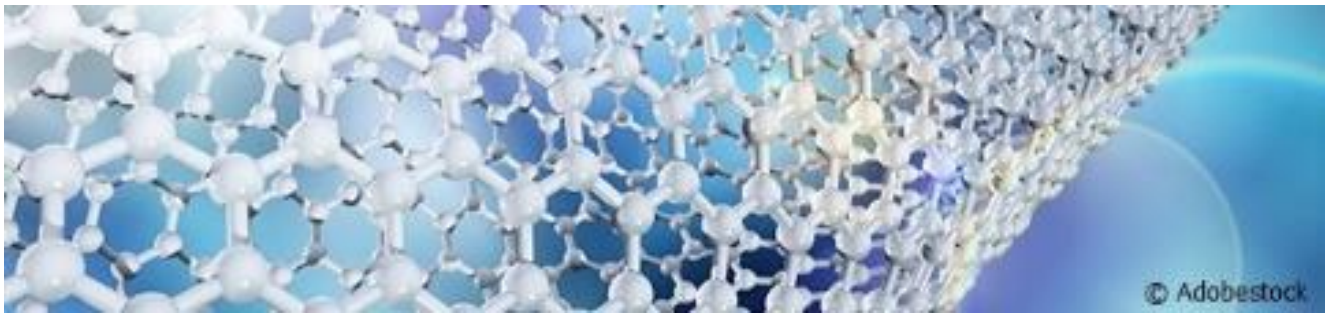


TOWARDS A PLURI / INTER / TRANSDISCIPLINARY

NEW AND SUSTAINABLE LIFE…

J. Yans[(1)]

(1) Department of Geology, Institute of Life-Earth-Environment, Transitions, University of Namur

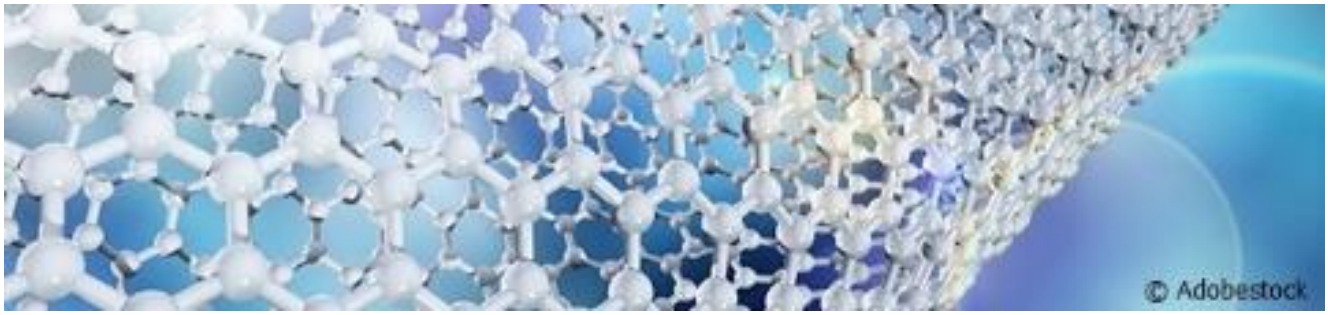
Our colleague Philippe Lambin is famous for his robust activities and prestigious career in the field of nanostructures. More recently (always?) he paid attention to sustainable development and development cooperation.

He organized the meeting "*Which Life? On an impoverished planet*" in 2008 at the Faculty of Sciences of the University of Namur, and initiated a transdisciplinary teaching of sustainable development at the University of Namur in 2015.

He is an active member of the *Group of Sustainable Development* at UNamur. He moreover developed research/cooperation dealing with the traceability/purification of coltan - (Fe,Mn) $(Ta,Nb)_2O_6$ -, geological ore from the artisanal mining in Democratic Republic of Congo – required (?) for the fabrication of mobile phones.

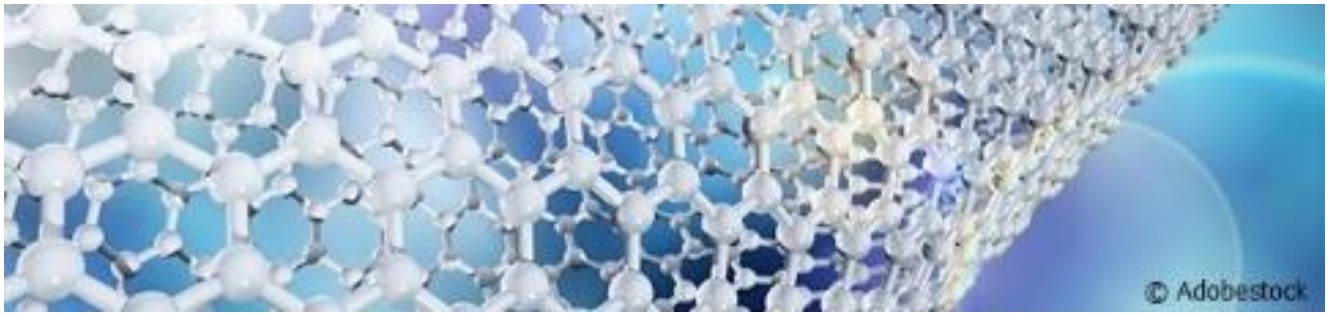
He is also a physicist with the soul of a poet…

NOTES…



Prof. PHILIPPE LAMBIN

Abstracts for POSTERS



DIAMETER-DEPENDENT OPTICAL ABSORPTION AND ENERGY TRANFER FROM ENCAPSULATED DYE MOLECULES TO SINGLE WALL CARBON NANOTUBES

Sofie Cambré[1], Stein van Bezouw[1], Jochen Campo[1], Joeri Defillet[1], Wim Wenseleers[1], Dylan H. Arias[2], Rachelle Ihly[2], Andrew J. Ferguson[2], Justin C. Johnson[2], and Jeffrey L. Blackburn[2]

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The hollow core and well-defined diameters of single-walled carbon nanotubes (SWCNTs) allow for creation of unique one-dimensional hybrid structures by encapsulation of various molecules. For instance, we previously demonstrated that in this way dipolar dye molecules can be naturally aligned in an ideal head-to-tail arrangement to create assemblies with a giant total nonlinear optical response.[1]

Here, we encapsulated specific dye molecules inside the SWCNTs and demonstrate that the optical absorption of the encapsulated dye molecules and subsequent excitation energy transfer (EET) from encapsulated dyes to the SWCNTs is strongly modulated by the SWCNT diameter, implying a diameter-dependent stacking of the molecules inside the SWCNTs.[2] The dye filling and EET are thoroughly characterized by optical absorption, resonant Raman, two-dimensional infrared photoluminescence excitation (PLE) spectroscopy and transient absorption spectroscopy.

In addition, we find that SWCNT filling does not limit the selectivity of subsequent separation protocols (including polyfluorene polymers for isolating only semiconducting SWCNTs and aqueous two-phase separation for enrichment of specific SWCNT-chiralities). The design of these functional hybrid systems, with tunable dye absorption, fast and efficient EET, and possibilities for subsequent separation, demonstrates potential for implementation in photo-conversion devices.

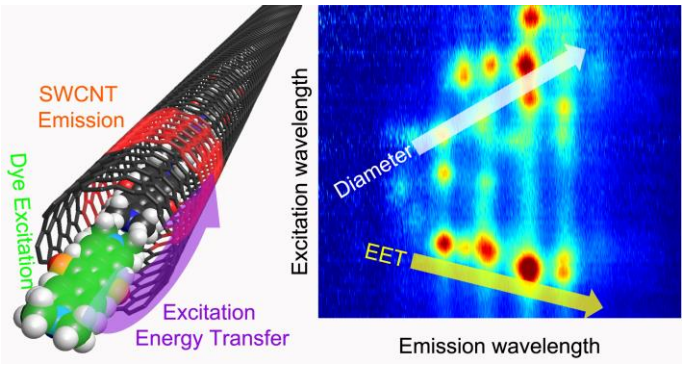

Fig.1 Excitation energy transfer from encapsulated dyes to SWCNTs probed by wavelength-dependent PLE spectroscopy.

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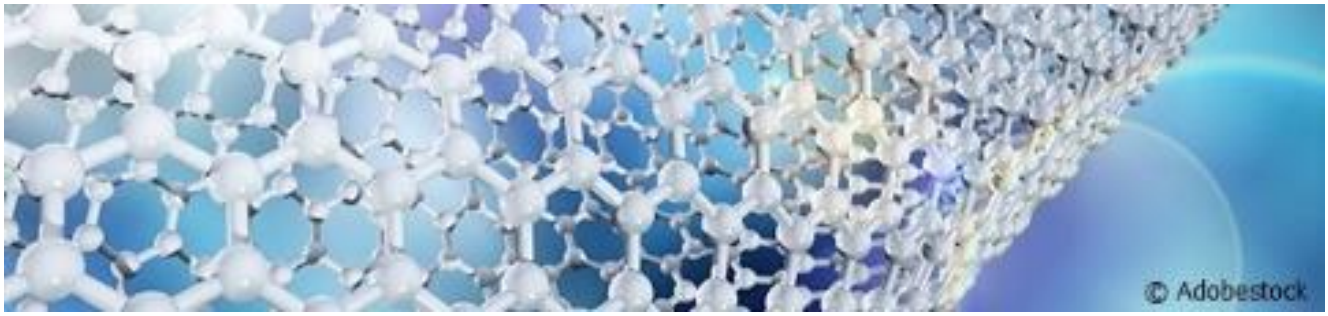

VIBRATIONAL SUM-FREQUENCY GENERATION (SFG) EXALTATION AT METALLIC INTERFACES

The cases of doubly resonant SFG in fullerene monolayers and of plasmon-enhanced SFG on metallic nanopillars

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Vibrational sum-frequency generation spectroscopy (SFG) is a second-order nonlinear optical technique that is intrinsically sensitive to the interfaces and boundaries of centrosymmetric materials. It combines an infrared (IR) laser beam (ω_{IR}) with a visible laser beam (ω_{VIS}) to coherently emit photons at the sum-frequency ($\omega_{SFG} = \omega_{IR} + \omega_{VIS}$). Since its invention three decades ago, SFG has proven extremely useful to investigate the structural order and the nanoscale organization of molecular thin films and surfaces. One drawback of the technique is the typically low intensity of the generated SFG beam, as it relies on a low-yield nonlinear optical process. In a classical SFG set-up, a resonance is observed in the SFG spectrum when the frequency-tuneable IR beam matches the oscillation frequency of a molecular vibration that is simultaneously infrared and Raman active. This presentation highlights two situations where large enhancements of the SFG intensity arise from electronic resonances that are jointly excited with molecular vibrations, by either the visible or the sum-frequency beam.

In the case of C_{60} fullerenes adsorbed on metallic surfaces, it was shown that the Raman-active "pentagonal-pinch" $A_g(2)$ vibration gains IR as well as SFG activity [1]: this is due to an interfacial dynamic charge transfer process, where electrons oscillate between the molecule and the metal substrate. Additionally, this mode SFG intensity is strongly enhanced when the SFG beam frequency is tuned to an intramolecular electronic excitation that is attributed to the HOMO – LUMO+1 transition [2]. This process is known as doubly resonant SFG (DRSFG). In the case of alkanethiol molecules self-assembled on metallic nanopillars grown on metal substrates, we evidenced that the SFG yield can be enhanced up to nearly three orders of magnitude [3]. This arises from the local field enhancement associated to the transverse and longitudinal localized surface plasmon resonances. The latter are resonantly excited by either the SFG or the visible beam. Our simple model of the SFG yield on these three-dimensional nanostructured interfaces explains why the enhancement is strongest for s-polarisation of the SFG and visible beams. This feature is rather counter-intuitive at first when considering metallic surfaces, where p-polarisation is usually the most sensitive to interfacial properties. For these two cases, the modelling of the underlying enhancement phenomena evidences their essentially different nature. Indeed, one is of intramolecular origin and involves a direct electron-vibration coupling mechanism (DRSFG), while the other one arises through indirect means (LSPR field enhancement).

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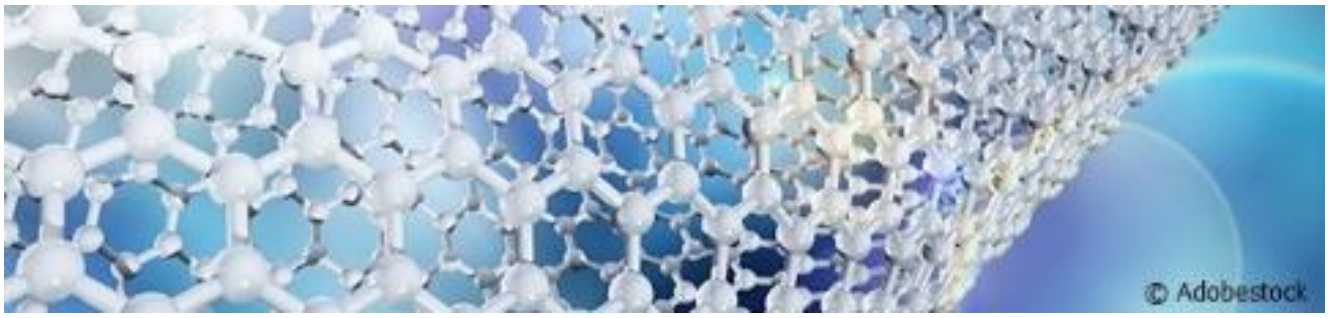
Acknowledgements: Y. C. and F. C. are research associates of the Belgian Fund for Scientific Research F.R.S.-FNRS. Part of this work was supported by the Walloon Region under the Waleo 3 project RAPARRAY. Y. C. wishes to thank Prof. Philippe Lambin for helpful discussions about fullerene physics and properties.



METHOD FOR PRODUCTION OF PLA-BASED MULTI-FUNCTIONAL NANOCOMPOSITES WITH IMPROVED PROPERTIES FOR 3D PRINTING APPLICATIONS

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The new properties of multifunctional polymer nanocomposites make them useful for a wide range of applications in a variety of fields such as space exploration, bioengineering, car production and organic solar cell development, etc. There is an unlimited need for new materials suitable for 3D printing for various applications that require improved mechanical properties, electrical, thermal conductivity and other functional properties of end products. The polymer matrix used in this study was Ingeo™ Biopolymer PLA-3D850 (Nature Works) grade developed especially for manufacturing 3D printer monofilament. Two types of carbon nanofillers were used: industrial graphene and multiwalled carbon nanotubes (TNIGNP, TNIMH4) and, respectively, those of higher quality (TNGNP and NANOCYL® NC7000 ™). Two procedures for preparing of PLA-based nanocomposites were applied using the melt mixing method by means of a twin-screw extruder: 1) Direct melt blending of the PLA polymer in the form of pellets with industrial carbon nanofillers and 2) Direct blending in the melt of the PLA in the form of powder with a higher quality carbon nanofiller. It was found that the PLA-based composites with graphene after the rheological percolation threshold of 6 wt% are optimal in terms of thermal conductivity. PLA based composites with MWCNTs obtained by the first procedure are optimal in terms of electrical conductivity around the rheological percolation threshold of 1.5 wt%. GNP-based composites, based on the first procedure are optimal in terms of electrical conductivity around the rheologically established percolation threshold of 6 wt%. PLA-based composites with MWCNTs obtained by the second procedure are optimal in terms of electrical conductivity around the rheological threshold of percolation below 1 wt%. A protocol for obtaining of filament for 3D printer, using a single screw extruder, has been optimized.

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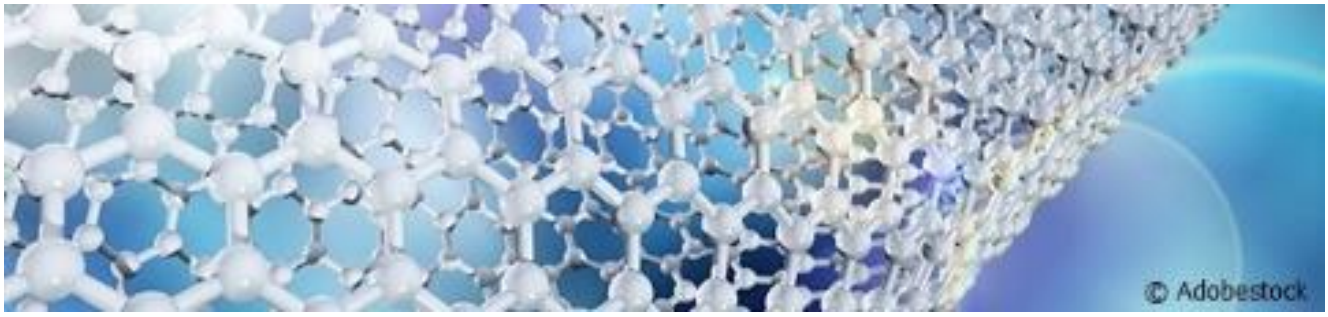

Multi-scale modelling of TCO coating deposited by reactive magnetron sputtering: application to structured c-Si thin film solar cells

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Transparent conductive oxides (TCO) present a large range of applications such as optoelectronic devices, especially transparent front-side contact for solar cells. In this last case, aluminium doped zinc oxide (ZnO:Al or AZO) can be a good alternative to indium doped tin oxide (ITO). However, the electrical and optical properties of such coatings highly depend on the structuration of the substrate. The present study focuses on nano-scale characterizations of AZO thin film deposited on micro-scale patterns.

The first step consists of nano-scale modelling of AZO deposition by reactive magnetron sputtering [1] on mono-crystalline silicone substrates thanks to a kinetic Monte Carlo model [2]. For these simulations, metallic (Zn, Al), reactive (O) and neutral (Ar) fluxes can be defined individually, with their own angular and energy distributions. Moreover, in order to mimic large samples, the periodic-supercell method is used. Then, electrical and optical characterizations of the coating can be performed. Electrical properties (effective electrical conductivity) are computed by the mean of a finite-element code solving the Maxwell-Faraday equation (hypothesis: near absence of varying magnetic field). Optical properties (effective optical index) are evaluated by using effective medium models (Maxwell-Garnett and/or Bruggeman). During all the process, a special attention is given to the substrate shape.

The second step is based on a micro-scale modelling of a full multi-layered structured c-Si thin film solar cell. The optical characterization (optical efficiency, short circuit current density) is done by RCWA [3] allowing to predict complex optical phenomena like scattering or light trapping. The major novelty of such study is the introduction in the RCWA simulation of the effective refractive indices of AZO depending on the position on the substrate (flat or tilted section of the pattern).

Finally, a full optimization by genetic algorithm [4] is performed in order to find the layer thicknesses and the pattern size parameters providing the best short circuit current density.

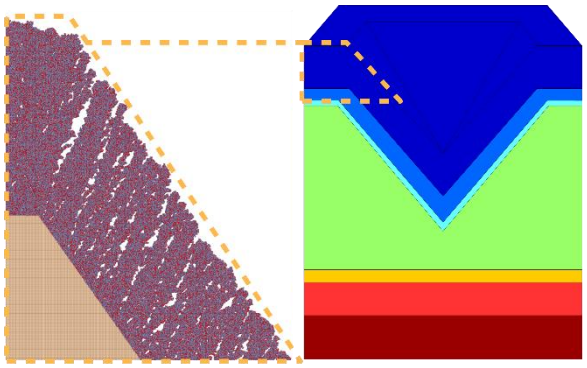

Figure 1: multi-scales modelling. Left: AZO coating on structured c-Si. Right: modelled solar cell.

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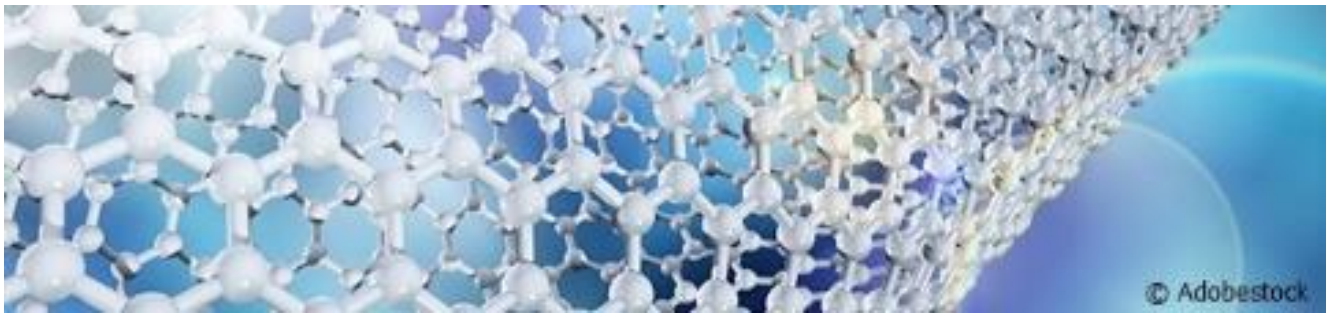

ELECTRONIC RAMAN SCATTERING IN INDIVIDUAL DOUBLE-WALLED CARBON NANOTUBES

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Double-walled carbon nanotubes (DWCNT), consisting of two coaxial and weakly van der Waals- coupled carbon layers, are one of the most ideal and fundamental systems to study the effects of interwall interaction on the physical properties in one-dimensional structures [1]. The properties of DWCNTs are related to (i) the nature of each of the constituent single-walled carbon nanotubes, which can be either metallic (M) or semiconducting (SC), and the combination type of the outer and inner tubes, i.e., SC@SC, SC@M, M@SC, or M@M; (ii) the van der Waals interactions, depending on the wall-to-wall distance, typically ranging from 0.33 to 0.42 nm; and (iii) the matching of the atomic lattices of the inner and outer tubes (Moiré patterns), which plays a decisive role in determining the electronic structure of a DWCNT even without any commensurability. The unique structure of DWCNTs offers advantages and opportunities for extending our knowledge and applications of the carbon nanomaterials family.

Here we report the measurement of the Electronic Raman Scattering (ERS) signal in individual structure-identified DWCNTs for the first time. The samples of individual suspended DWCNTs were obtained by means of catalytic chemical vapor deposition and examined carefully by a combination of electron diffraction, high resolution transmission electron microscopy, Rayleigh and Raman scattering spectroscopies at different excitation wavelengths [2]. The effect of the interwall coupling on the ERS signal has been analyzed. Future possible applications of this phenomenon in the field of DWCNTs characterization are discussed.

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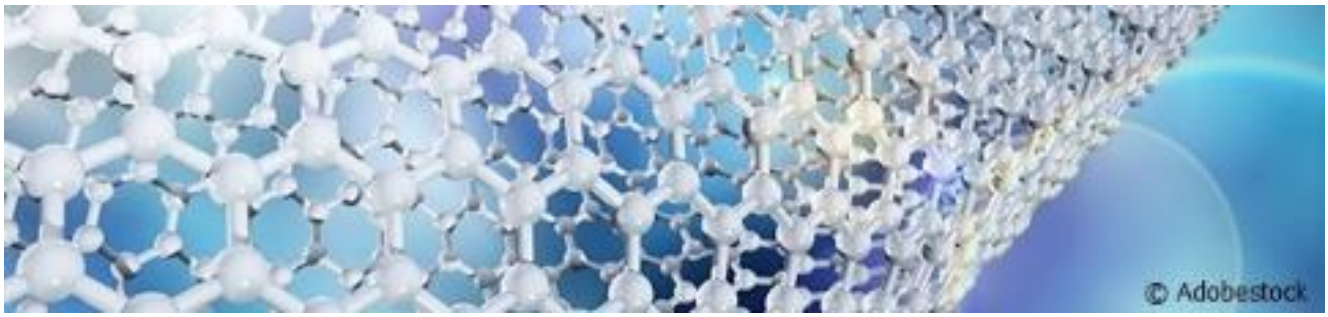

MASSLESS FERMIONS IN 3D CARBON STRUCTURES

the missing Dirac cone

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The discovery of massless Fermions in low-dimensional carbon-based nanostructures has strongly impacted condensed matter physics by introducing pseudo-relativistic effects in their electronic properties. Indeed, the linear energy dispersion with the crossing of electronic bands at a particular point, forming the so called Dirac cone, imposes the electrons to behave like massless Dirac Fermions in graphene (2D) and carbon nanotubes (1D). Intense efforts have been realized to extent the tremendous properties of massless Dirac Fermions to the 3D materials family. Recently, massless Fermions have been experimentally evidenced in several 3D materials such as Na3Bi [1], Cd3As2 [2,3] and HgCdTe [4] paving the way towards a new class of materials.

In the present work, we predict the possibility to observe 3D massless Dirac Fermions in a schwarzite structure (Fig.1), a 3D purely carbon-based allotropic form [5]. Carbon schwarzites consist of a graphenic surface in which carbon rings with more than six atoms (heptagons, octagons, etc.) are incorporated to induce negative curvature. By means of density functional theory and tight-binding approaches, the electronic properties of a large gyroidal schwarzite structure are investigated. Fully isotropic and symmetric linear band crossings are evidenced. The corresponding charge carriers are thus expected to behave as 3D massless Dirac Fermions. This schwarzite can thus be considered as a remarkable playground to investigate the physics of these exotic Fermions in 3D materials.

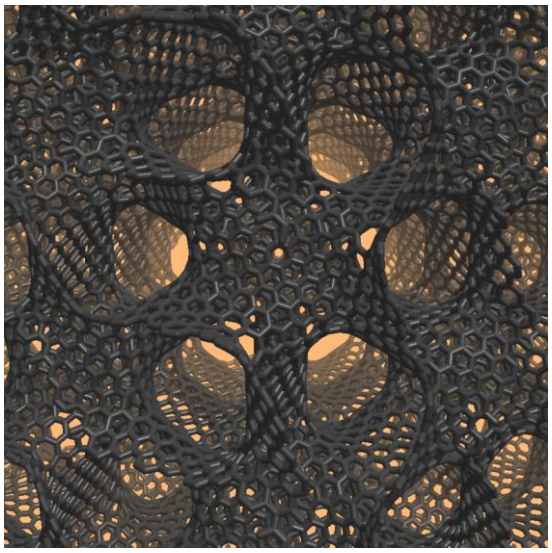

Figure 1: Atomic model of a carbon-based 3D schwarzite structure

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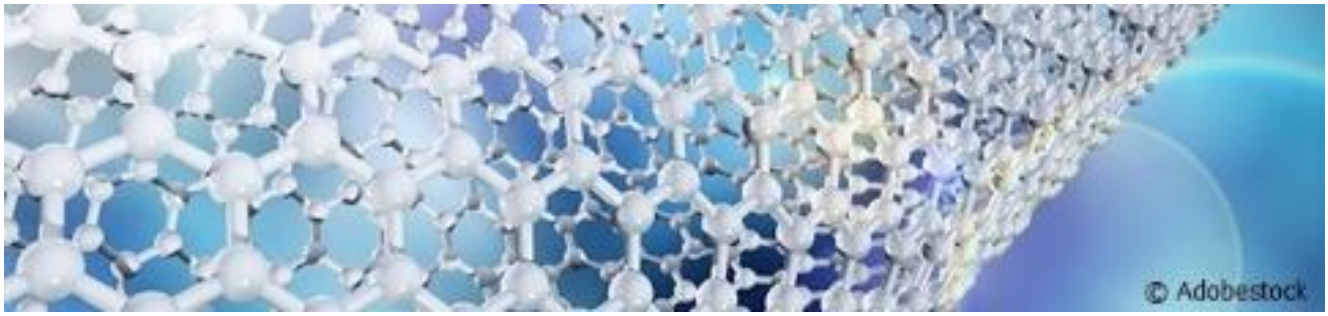

CONTROLLED FLUORESCENCE IN THE PHOTONIC STRUCTURE OF *EUPHOLUS LINNEI WEEVIL'S SCALES*

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The optical structures found in some weevils' scales are generally associated with photonic crystals [1-4]. These structures are periodic along one, two or three dimensions. Such periodicities affect the propagation of electromagnetic waves inside the structured material through light interference. In addition to these optical effects, fluorescence emission can also occur in beetles' scales due to the presence of fluorophores which are naturally embedded within the structures' materials [3].

This phenomenon is however underinvestigated. In this study, we analysed the fluorescence emission controlled within *Eupholus linnei* weevil's 3D photonic structures. This beetle is characterised by turquoise-striped black elytra. The turquoise colour of these stripes is due to scales exhibiting various photonic domains ranging from orange to blue under incident white light.

Under ultraviolet light, the turquoise stripes emit light in the visible spectrum. Using electron microscopy, 3D photonic structures were found in the weevil's scales. In addition to spatial measurements of the scales' reflectance and the analysis of these scales' colours in terms of chromaticity, the optical response of the observed nanostructures was modelled and predicted using the dominant reflected wavelength formula as well as optical simulation methods such as the Rigorous Coupled-Wave Analysis (RCWA) [4].

Furthermore, the fluorescence properties of the scales were measured by spectrofluorimetry. The related decay time was evaluated to be longer at a wavelength within the photonic bandgap of the structures than outside this photonic bandgap. The quantum yield of the fluorescent scales was estimated to be rather low (about 21%), suggesting that fluorescence emission does not play a role in the visual appearance of the investigated weevil.

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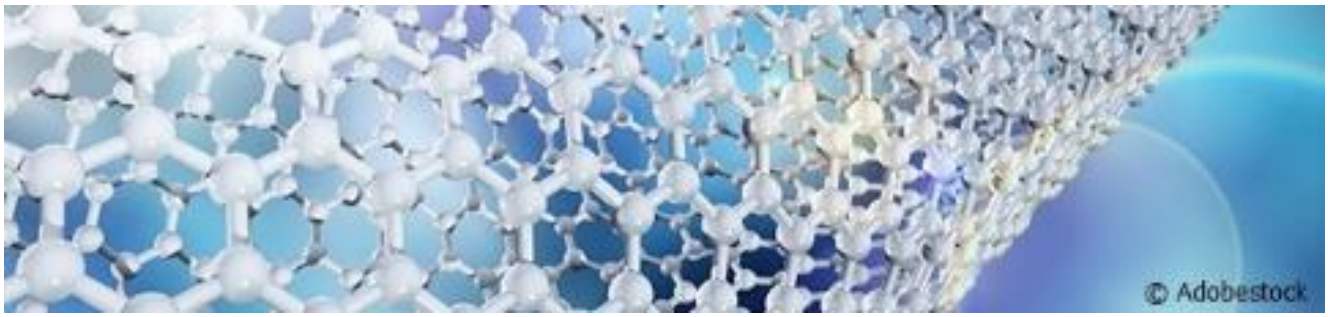

ELECTROMAGNETIC PROPERTIES OF MONO- AND MULTILAYERED 2D MATERIALS: APPLICATION TO GRAPHENE

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Electromagnetic properties of 2D materials are of primary interest in a range of applications such as biosensing, transparent conductor, shielding or optronics. They have been modeled either as a thin film with an effective volume permittivity or as a single sheet with a surface conductivity. However, discordances have been recently reported in the analysis of the optical properties depending on the model.

Here, we fully account for the particular anisotropy of 2D material and reconcile both approaches. We propose a unified description of the electromagnetic properties that applies to 2D heterostructures for both polarizations and all angles of incidence. In particular, we analyze the class of materials for which both models can be used indifferently or when particular care should be taken to the thickness and tensorial response of the effective thin film [1].

We also propose a new method to experimentally deduce the surface conductivity of a 2D material. This method is based on the optical measurement of the Brewster angle when a conducting 2D material lies on a dielectric substrate. We exemplified our proposal by ellipsometry measurements on CVD grown graphene with controlled number of layers. [2]

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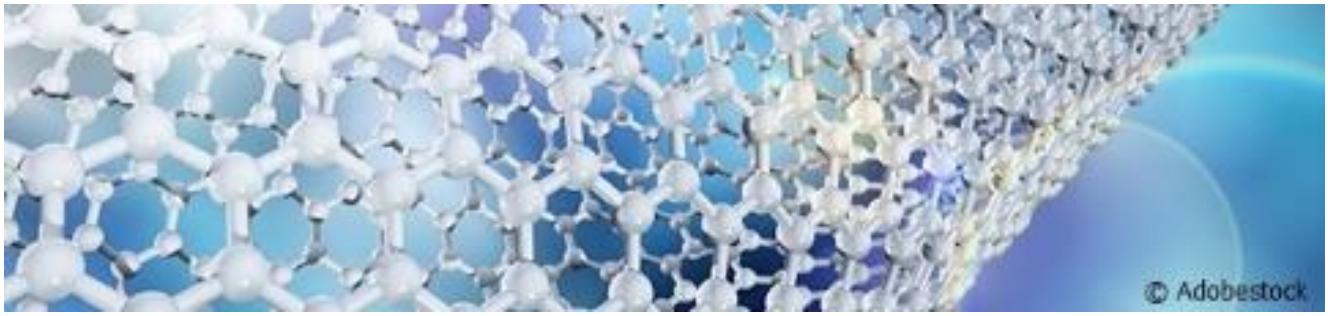

Wave packet dynamical simulation of defects in 2D materials

The Huygens principle and the band structure

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One of the possible material families of the post-Silicon era is the family of the two dimensional (2D) materials. Wave packet dynamics (WPD) is a flexible method to simulate electronic dynamics and transport phenomena at the nanoscale which is capable of calculating realistic models containing several hundred atoms. Dispersion relations calculated by density functional (DFT), or other state of the art methods make it possible to extend wave packet dynamical calculations for virtually any crystalline material. This is because the E(k) dispersion relation contains the full electronic structure information for a given crystalline material. We constructed formerly a general method[1] to include the band structure information into the WPD calculation. Real materials, however, are newer perfect crystals, they contain various structural defects. Effect of the local defects can be incorporated into the dispersion relation based wave packet dynamical calculation by introducing local potentials. This is illustrated on Fig. 1, which shows snapshots of a WPD simulation for a graphene surface having a local defect. The WP is injected (e.g. from a tip of a Scanning Tunneling Microscope) in the middle of the image. Figure 2. shows the difference wave function. We can see that the local potential causes a scattering with hexagonal symmetry.

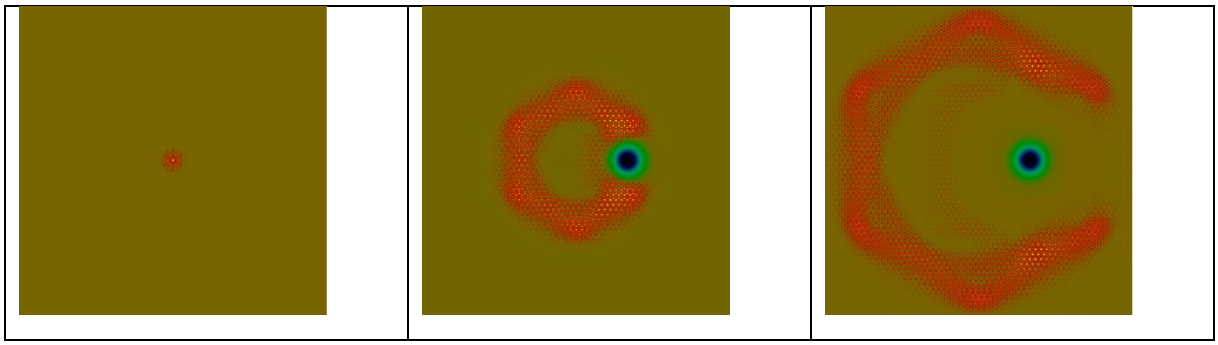

Figure 1. Snapshots of the time development of the probability density of a wave packet spreading on graphene surface. The wave packet starts from the centre. The local potential is shown by a large dark dot.

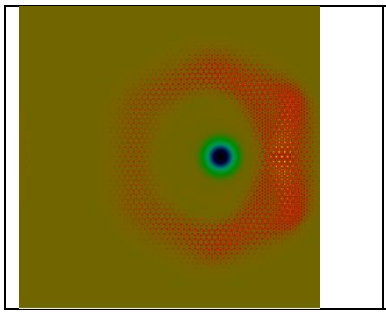

Figure 2. Probability density of the difference wave function, $\left|\varphi_{with\,pot} - \varphi_{free}\right|^2$. This wave function shows a scattering dictated by a "modified Huygens principle" – the local scattering has a hexagonal pattern, because of the anisotropic nature of the graphene dispersion relation (trigonal warping effect).

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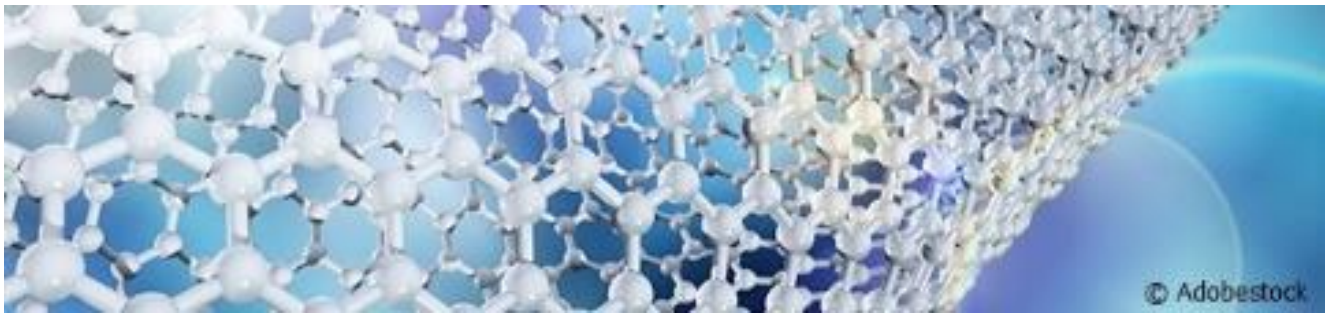
Acknowledgements:

Valuable discussions with Ph. Lambin and A. Mayer of University of Namur are gratefully acknowledged.



A CHARGE-DIPOLE MODEL TO COMPUTE THE POLARIZATION PROPERTIES OF CARBON NANOTUBES AND FULLERENES

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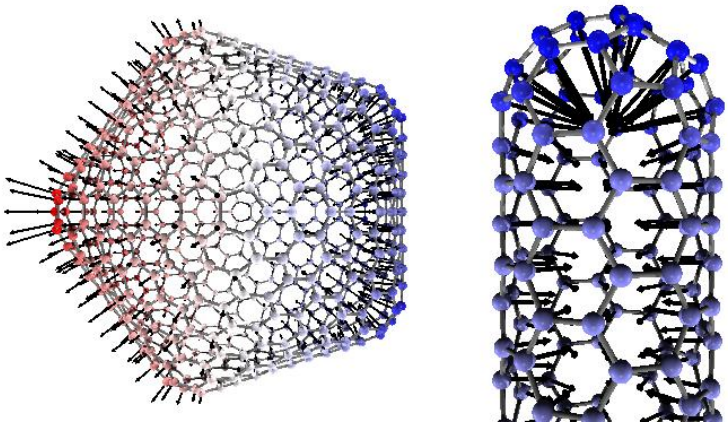
In order to compute the polarization properties of fullerenes and carbon nanotubes, we present a model in which each atom is represented by both a net electric charge and a dipole. The consideration of net electric charges enables one to address the fact that electrons move from one part of the molecule to another in response to an external field. It also enables one to account for the accumulation of extra charges.

These effects, which actually occur in any metallic structure, are poorly accounted for by models that rely on dipoles only. We propose here a computational scheme to determine these atomic charges and dipoles. It is based on the requirement that the total electrostatic energy of the system is minimized. The use of normalized propagators for the electrostatic interactions between the atomic charges and dipoles gives the model both a better consistency and an improved numerical stability.

The model can be easily extended to structures made of different types of atoms. An extension that enables the computation of frequency-dependent polarizabilities was also developed. The idea consists in relating the time variations of the atomic charges to the currents that flow through the bonds of the structure considered. The atomic charges and dipoles are then determined by a least-action principle.

This model was applied with success to the computation of the molecular polarizability of fullerenes, carbon nanotubes, alkanes, alkenes, aromatic molecules and silver clusters.



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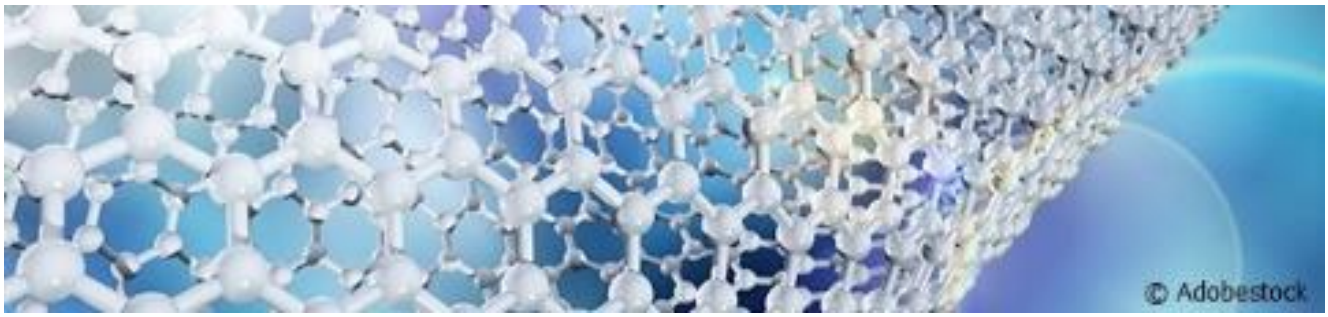

NON-LINEAR AND LINEAR OPTICAL PROPERTIES OF A BEETLE'S FLUORESCENT PHOTONIC NANOSTRUCTURES

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Fluorescence emission occurs in the integuments of many natural species including but not limited to insects, arachnids, mammals, anthozoans (e.g., sea anemones and corals) and scyphozoans (i.e., true jellyfish). In insects, fluorophores, such as papiliochrom II and biopterin, are at the origin of such light emission. In some cases, they are naturally embedded in photonic nanostructures, which influence the emission in terms of spectral intensity, decay time and spatial distribution [1,2]. Using linear and non-linear optical and fluorescence techniques, the case of the *Hoplia coerulea* male beetle was investigated. The photonic structures found in the scales covering its body comprise fluorophores. These structures control both the insect's colouration and the emission from the embedded fluorophores [2,3]. Contact with liquids gives rise to variations of the emission properties. The combination of these observations and optical modelling allows the study of the photonic confinement within the beetle's nanostructures. Additionally, Third-Harmonic Generation and two-photon fluorescence analyses unveiled the multi-excited states character of the fluorophores and, through light polarisation effects, the role of the photonic structures' anisotropy in the fluorescent behaviour [4]. In addition to the elaboration of new concepts and the development of technological applications through a bioinspiration approach, such investigations help the understanding of the biological functionalities behind the observed fluorescence response.

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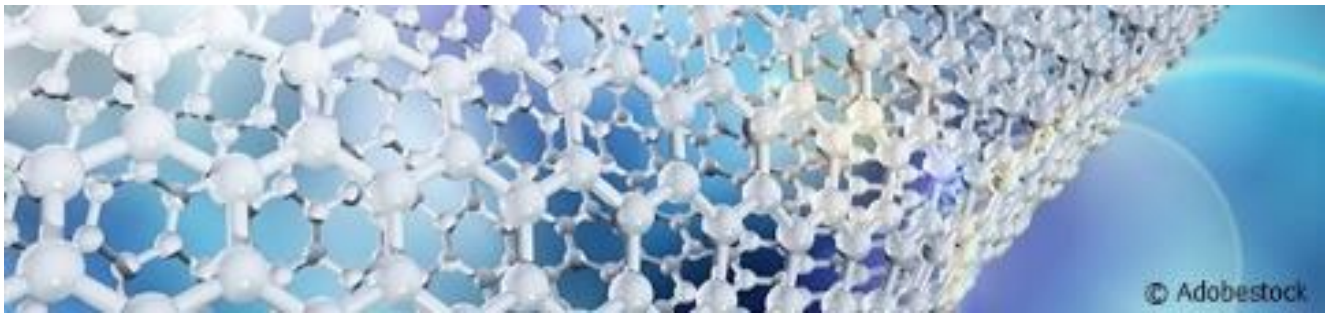

Kivu's coltan: A facility for chemical-physics treatment and application study

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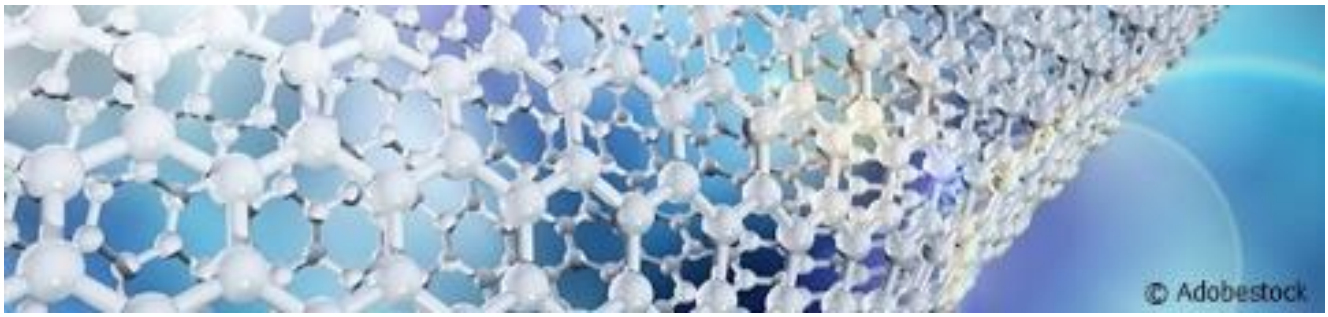
Coltan is a mineral from which tantalum (Ta) and niobium (Nb) can be extracted, among other metals. In this black ore, Ta and Nb are present in the form of tantalite (Ta_2O_5) and colombite (Nb_2O_5). In addition to many applications in metallurgy, tantalum has become an important element for the fabrication of electrolytic capacitors used in modern electronic circuits. In a Ta capacitor, the very thin oxide layer that serves as dielectric spacer (permittivity constant about 27) between the Ta anode and a surrounding electrolyte makes it possible to reduce the overall size while keeping the same capacity as that of capacitors made with other materials. This is why Ta capacitors are essential components in miniaturized circuits used in today portable electronic devices.

The exponential-like increase of such devices exerts a strong pressure on the Ta market. The price of this metal does not increase in proportion to the demand, because tantalite is made available for almost nothing from raw mines in the Eastern border of the Democratic Republic of Congo. Minors are working there days and nights, in total insecurity and for a miserable salary. Local cooperatives that collect the extracted coltan have only a rough estimate of the exact composition of the minerals that are eventually sold to bigger entities, often for an arbitrary price.

The aim of the project is to install and develop a laboratory for the characterization and purification of the extracted coltan. The laboratory will be based in the *Institut Supérieur Pédagogique de Bukavu* in South Kivu. Local characterization of samples will be made by X-ray fluorescence analysis using a portable equipment. In parallel, an experimental small-scale plan for purification will be designed and tested under local environment conditions (regular power cuts, absence of pure water …). Photovoltaic cells will be installed to supply the laboratory with electricity.

The purification consists in a physical separation process, followed by a chemical digestion of the mineral matrix in acids at 100°C. The obtained metal salts will finally be collected in specific solvents. Purified samples will have a much higher commercial value on the market, which in the long run should contribute to improve the life conditions of all the actors involved in the coltan circuit, especially and hopefully at the level of the so-called “extractors”. In parallel, an educational program led by the Catholic University of Bukavu, will target female workers who still are present in the heart of mines. With a suitable education, women will hopefully be in position to stop any hard mining activity to take up more administrative duties in mine cooperatives. Finally, fundamental research will be conducted in the *Institut Supérieur Pédagogique de Bukavu* on the properties and possible applications of Ta and Nb-based perovskites as possible multiferroic compounds.



KLEIN TUNNELING AND ELECTRON OPTICS IN DIRAC-WEYL SYSTEMS WITH TILTED ENERGY DISPERSION

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The outstanding electronic and transport properties of relativistic-like fermions have been extensively studied in solid state systems with isotropic linear dispersions such as graphene [1]. Among many interesting phenomena discovered, the Klein tunneling is a direct evidence and concurrently provides a playground for implementing tests of relativistic quantum dynamics of quasiparticles in simple experiments [2]. In addition, the Dirac fermions in graphene exhibit several behaviors analogous to light rays in optical media [3] such as refraction, reflection, and Fabry-Pérot interferences, making it an ideal platform for electron optics demonstration and novel quantum device development.

Beyond graphene, several (both 2D and 3D) Dirac-Weyl materials have been recently explored [4]. In contrast to graphene, many of them however exhibit tilted (and also anisotropic) energy dispersions around the Dirac-Weyl cones, leading to novel electrical and optical phenomena.

In this talk, we present novel transport properties of Dirac-Weyl fermions in hetero-doped structures [5] induced by the effects of tilted energy dispersion. In particular, we find that instead of being observed in a unique direction (i.e., normal incidence) as in the non-tilted case, the Klein tunneling of tilted Dirac-Weyl fermions of opposite chiralities is achieved in two separated oblique directions. In addition, interesting phenomena such as anisotropic Fabry-Pérot resonances, valley filtering and beam splitting effects, and novel electron optics behaviors in Dirac-Weyl p-n junctions are also predicted. Besides being crucial to fully understand the relativistic-like phenomena of Dirac-Weyl fermions, our findings could be the basis for novel applications of the host materials in electron optics and valleytronics.

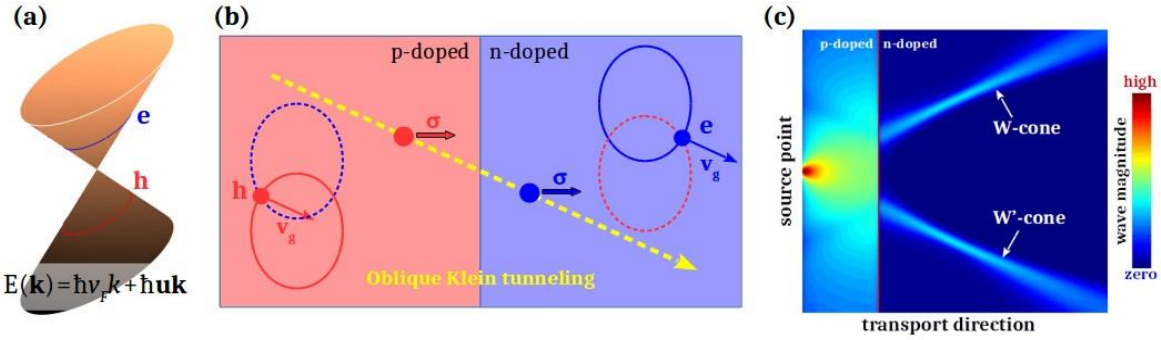

Fig.1: Transport properties of Dirac-Weyl fermions with tilted energy dispersion in hetero-doped systems. (a) Tilted Dirac-Weyl energy dispersion. (b) A diagram illustrating the observed oblique Klein tunneling: □ pseudospin and vg group velocity. (c) Dirac-Weyl fermion wave propagating through a p-n doped interface.

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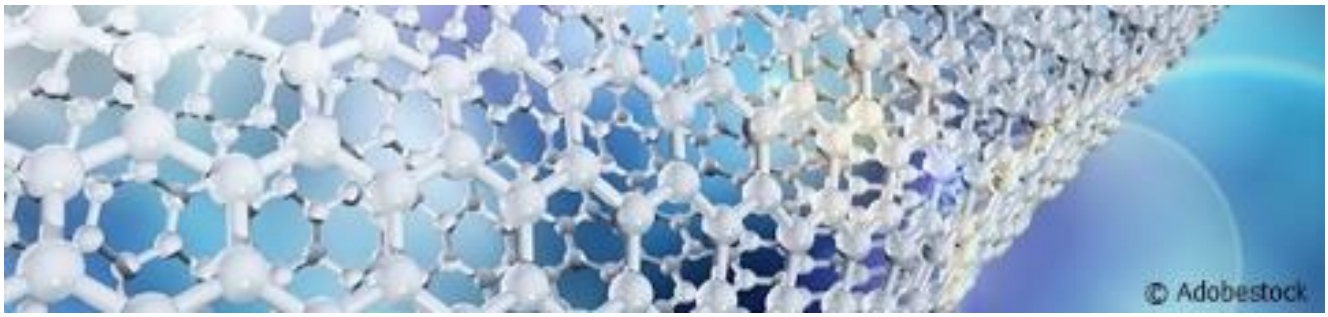

RAMAN SPECTROSCOPY OF DOUBLE-WALLED CARBON NANOTUBES

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Double-walled carbon nanotubes (DWNTs), consisting of two coaxial and weakly van der Waals coupled single-walled carbon nanotubes (SWNTs), are one of the most ideal and fundamental systems to study the effects of inter-tube coupling on the physical properties in one-dimensional structures.

On this poster, we report on the investigations of individual, spatially isolated and suspended double-walled carbon nanotubes (DWNTs) by combination of high-resolution electron microscopy, electron diffraction, Rayleigh spectroscopy and Raman spectroscopy [1,2]. We first present an overview of the effect of the diameters, inter-tube distance and nature (metallic or semiconducting) on the Raman signature (Radial Breathing Like [1,3,4] and Tangential Modes [4-6]) of DWNTs.

We then examine the features of tangential modes and find a clear frequency shift of the inner-layer G modes as a function of the inter-tube distance with respect to the corresponding G modes in equivalent single-walled carbon nanotubes (SWNT).[4-6] These results are understood by considering the effects of the relaxation of the layers and the interaction between the relaxed structures.[7] Finally, we study the experimental excitation dependence of the G modes intensity of the constituent inner and outer SWNTs. In particular, we discuss the effects of the quantum interference between different electronic transitions on the observed behaviours.[8]

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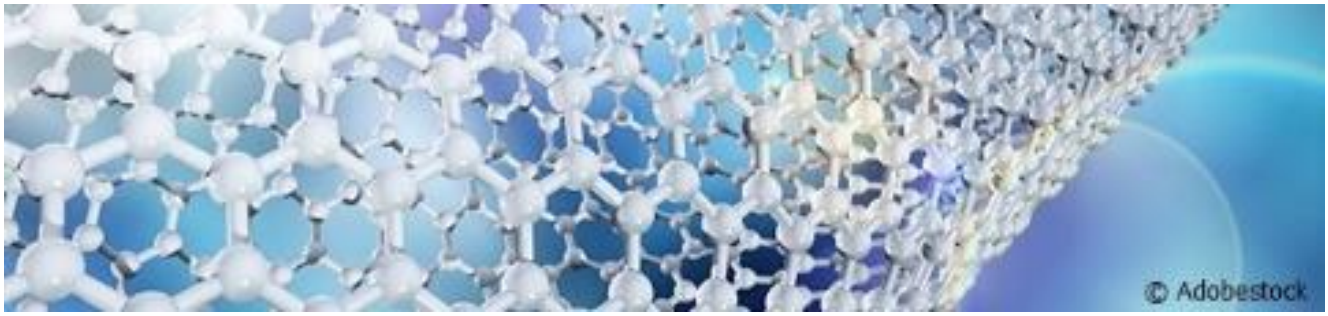

ROBUSTNESS OF ENTANGLEMENT TRANSMISSION WITHOUT PLASMONIC RESONANCE

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We studied the survival of quantum entanglement after the interaction of polarization-entangled photons with a flat, thin film of polycrystalline gold, for different angles of incidence (0°, 20°, 35°, 50°). The near-infrared (818 nm) polarization-entangled photons pairs are produced by parametric downconversion using two identical type-I BBO-crystals with orthogonal optical planes. The sample is placed through the path of one of the photons of the produced pairs. In each photon path, quarter and half waveplates placed in front of a polarizing beamsplitter select the basis of the polarisation measurement. Photons are finally detected with four single-photon counting modules and coincidences are recorded using a field-programmable gate array coincidence counter. We use the code developed by Paul Kwiat's quantum information group [1] to realise quantum tomography of the polarization-entangled photons with and without the sample, in order to determine of the quantum state of the pairs before and after their interaction with the thin gold film. With this estimation of the quantum state, we evaluated different quantum features of the system, like the entanglement of formation (σi), the experimental state fidelity with respect to the maximally entangled Bell state theoretically produced $F(\phi+, \sigma i)$, and the trace distance between the state obtained before and after the sample $DTr(\rho_0, \sigma_i)$. These properties quantify the influence of the planar film on the entanglement and polarization state of the photon pairs. Our experimental and theoretical results show that, at normal incidence, the sample does not affect the polarization of transmitted photons and, consequently, that entanglement is preserved even though the total number of detected correlations decreases. When increasing the angle of incidence, the different transmission coefficients for s and p polarisations decrease entanglement, as the sample starts to behave as a partially polarizing device. This effect is negligible up to 20° of incidence. We also studied similarly a periodic array of subwavelength nanostructures on a metallic film. As shown in the literature [2–4], such materials enable coupling of light with localized surface plasmons: they allow greatly enhanced transmission at resonance with preservation of entanglement. In comparison to nanostructured samples, our results on the flat, thin film of gold indicate that the interaction with surface plasmons at resonance enhances transmission. However, it does not play a role on the robustness of the quantum entanglement for the photon pairs that are transmitted: it only improves the rate of the correlation detection.

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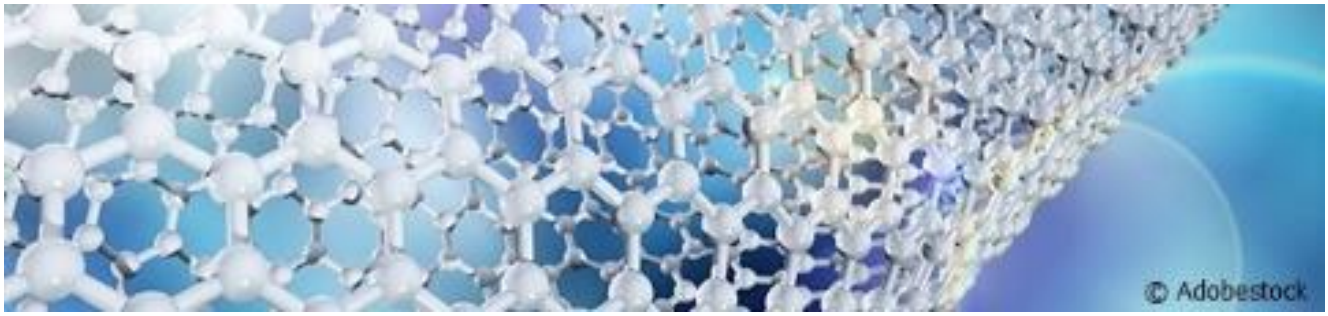

First-principles investigation of 2D lattice coherency in van der Waals heterostructures

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Beginning with graphene-hBN van der Waals (vdW) heterostructures [1], many Moiré patterns between 2D materials have been observed [2,3]. Still, predicting the coherent, semi-coherent (Moiré) or incoherent matching of 2D lattices at their interface is a challenge for Density Functional Theory (DFT), due to the very large size of the supercells needed in such studies. We introduce a first-principles-based model that bypass the need for large supercells. It generalizes the well-known Frenkel-Kontorova model [4] by including physical effects present in real materials, as derived from a perturbative approach to the problem. In particular, a mean-field modification of the 2D lattice parameters and elastic constants appears, even if the matching of the lattices is incoherent. The results are compared to plain DFT computations and to experimental observations of lattice accommodation in vdW-heterostructures. Then, we predict lattice (in)coherency for a set of 36 vdW-heterostructures based on graphene, phosphorene and different transition metal dichalcogenides.

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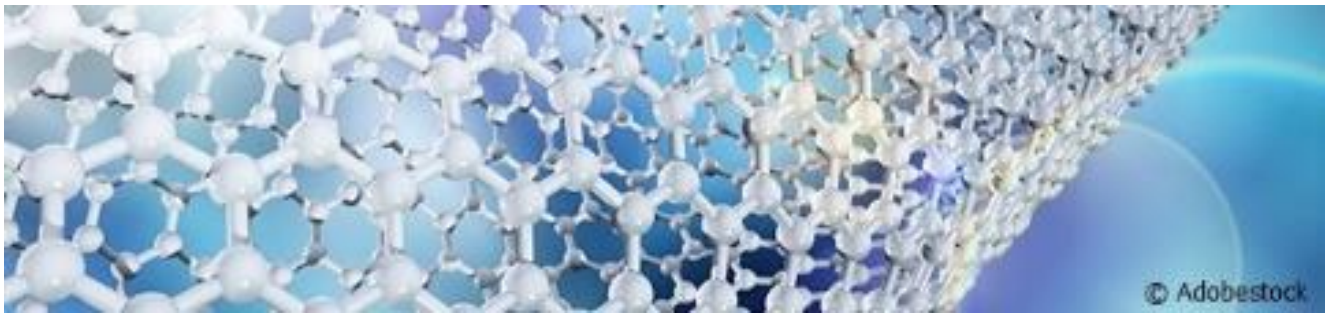

DEFECTS RELATED PROPERTIES IN TWO-DIMENSIONAL MOS_2

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As already demonstrated for graphene, an important issue in 2D materials is the presence of defects, which can significantly influence their electronic, magnetic, or optical properties with a direct impact on applications. In this work we provide atomic level insights into the properties of point defects (0D) and line defects (1D) of single layers MoS_2 by using electronic structure calculations combined with atomic resolution Scanning Tunneling Microscopy (STM) measurements. We found that sulfur vacancy is the most common point defect in MoS_2 which causes localized midgap states in the band gap [1]. Furthermore, STM measurements revealed that under ambient conditions oxygen gradually incorporates into the basal plane of the MoS_2 crystals through a substitutional oxidation reaction, by replacing individual sulfur atoms. The resulting 2D $MoS_{2-x}O_x$ solid solution crystals are characterized by catalytically active basal planes, where substitutional sites can be identified as active reaction centers, increasing the catalytic activity for electrochemical H_2 evolution reaction [2]. In the case of the line defects, we have investigated the magnetic properties of zigzag edges of several nanometer long MoS_2 nanoribbons by using the Hubbard model. The results predict low domain wall energies along the edges, which are also sensitive to the presence of edge disorder. Our theoretical and experimental results give an insight into the properties of defects in MoS_2 and can also provide valuable information for catalytic and spintronic applications.

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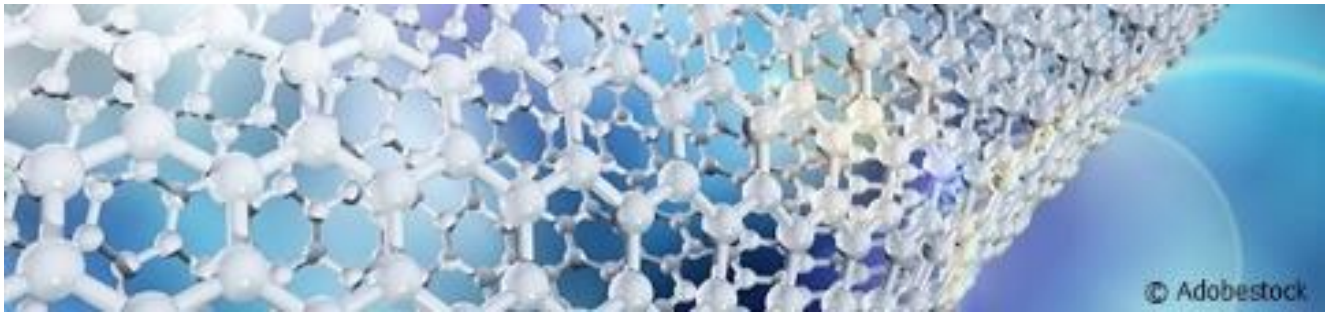

SINGLE FILES OF DIPOLES ALIGNED IN CARBON NANOTUBES:

Building blocks with giant nonlinear optical response

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Asymmetric dye molecules, acting as electric 'rectifiers' with a large second-order nonlinear optical (NLO) response (hyperpolarisability β), find applications in ultrafast electro-optic switches for optical telecommunication and wavelength conversion of lasers.[1] In 3D bulk materials, however, such dipolar molecules tend to align in a pairwise anti-parallel way, cancelling each other's directional properties, such as the NLO response.

We show that by encapsulating such elongated dipolar molecules in the 1D internal channel of single-wall carbon nanotubes (SWNTs), Coulomb interactions naturally favour a polar head-to-tail alignment of the molecular dipoles, leading to a coherent addition of their second-order NLO responses.[2] The encapsulation is evidenced by extensive wavelength-dependent fluorescence-excitation and resonance Raman experiments on bile-salt solubilized[3] dye-filled SWNTs, revealing the critical diameter for filling through the effect of encapsulation on the vibrational[4] and electronic[5] properties of the SWNTs and the encapsulated molecules.

The nonlinear optical response of the nanohybrids is characterized using a unique setup for wavelength-dependent hyper-Rayleigh scattering (i.e. second harmonic light scattering),[6,7] indeed showing that these organic-SWNT nanohybrids possess giant NLO responses, also allowing the domain size of head-to-tail aligned chromophores to be determined. Their equally giant total dipole moment and size promises an easy and stable alignment of the nanohybrids, opening an entirely new route towards the rational design of solution processable yet stable NLO materials.

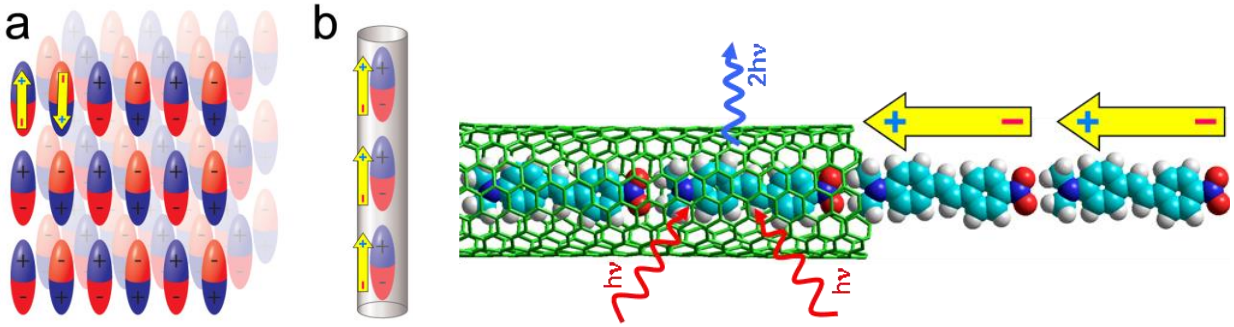

Figure 1. Alignment of asymmetric dipolar molecules in (a) a bulk material or (b) inside a SWCNT.

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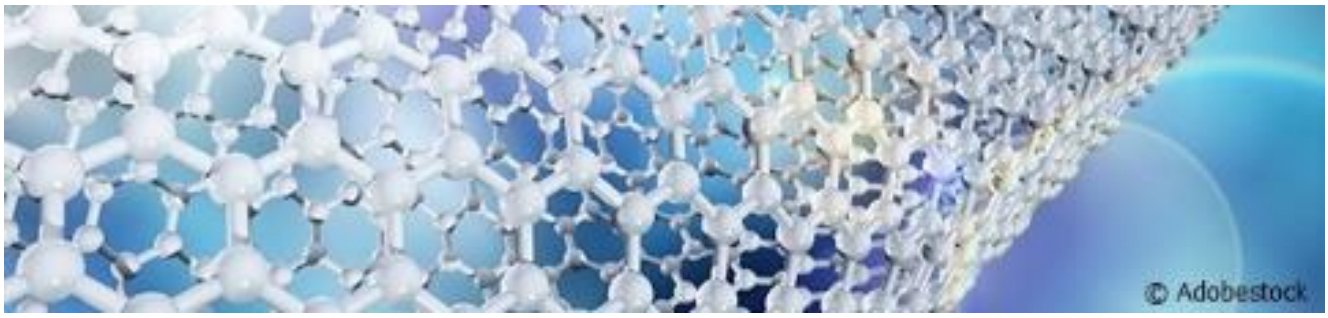

ELECTRONIC AND TRANSPORT PROPERTIES OF SINGLE AND DOUBLE WALL CARBON NANOTUBES

N. Wittemeier

ICN2: Catalan Institute of Nanoscience and Nanotechnology

Carbon nanotubes haven been studied thoroughly since their discovery in 1991[1], revealing a variety of electronic properties, that depend strongly on the exact structural composition of the nanotube. In recent experiments, measuring the transport gap in multi-wall carbon nanotubes, negative differential conductance has been observed [2].

Simulations of single and double-wall carbon nanotubes (DWNT) with first-principle methods have been performed and used to set up a tight-binding model that accurately describes inter- and intra-layer interactions. Utilizing the scalability of the tight-binding model as well as non-equilibrium green-functions methods, transport gaps in DWNTs with semiconducting outer shells have been investigated in order to search for negative differential conductance and identify the underlying mechanism.

The simulations reproduce general transport properties of carbon nanotubes without observing any negative differential conductance, indicating that the phenomenon is not of purely electronic nature.

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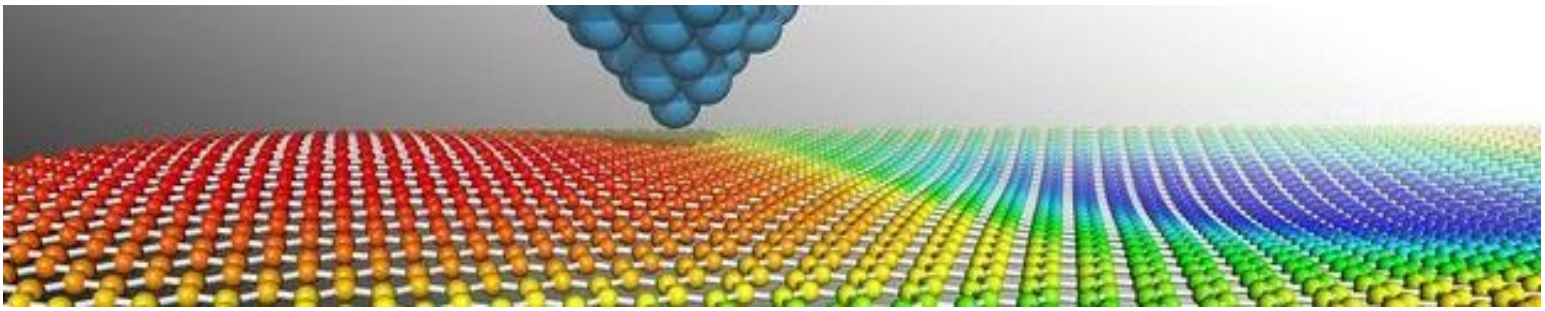

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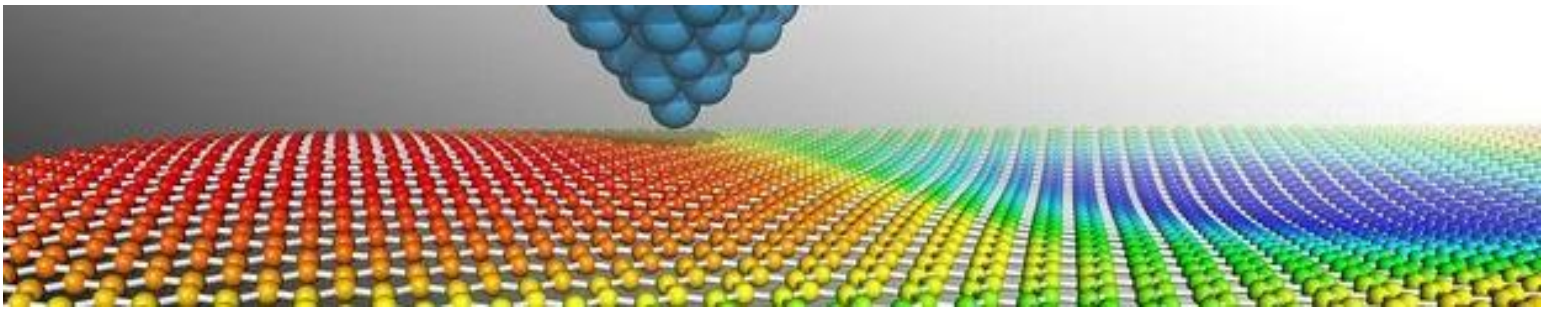

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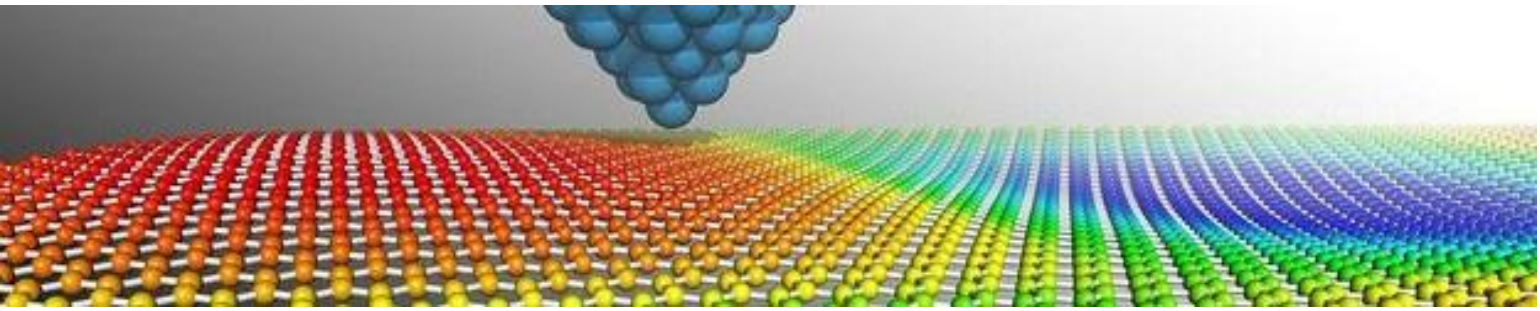

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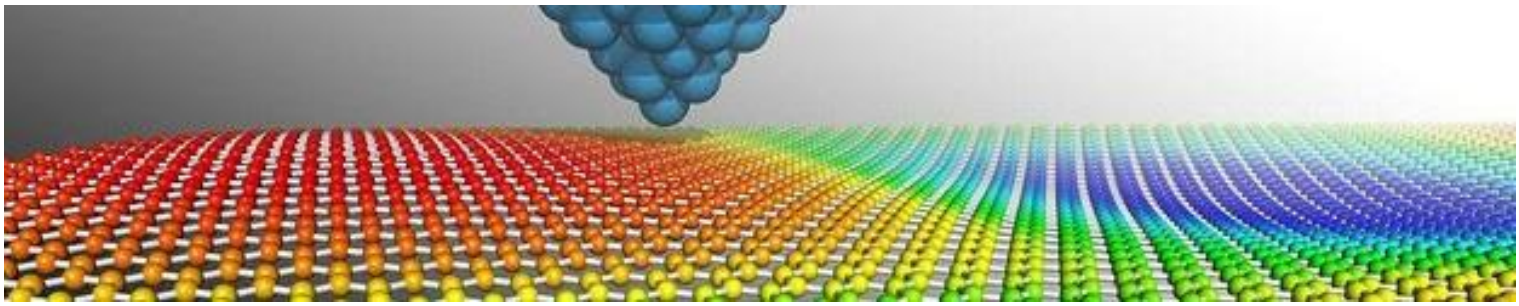

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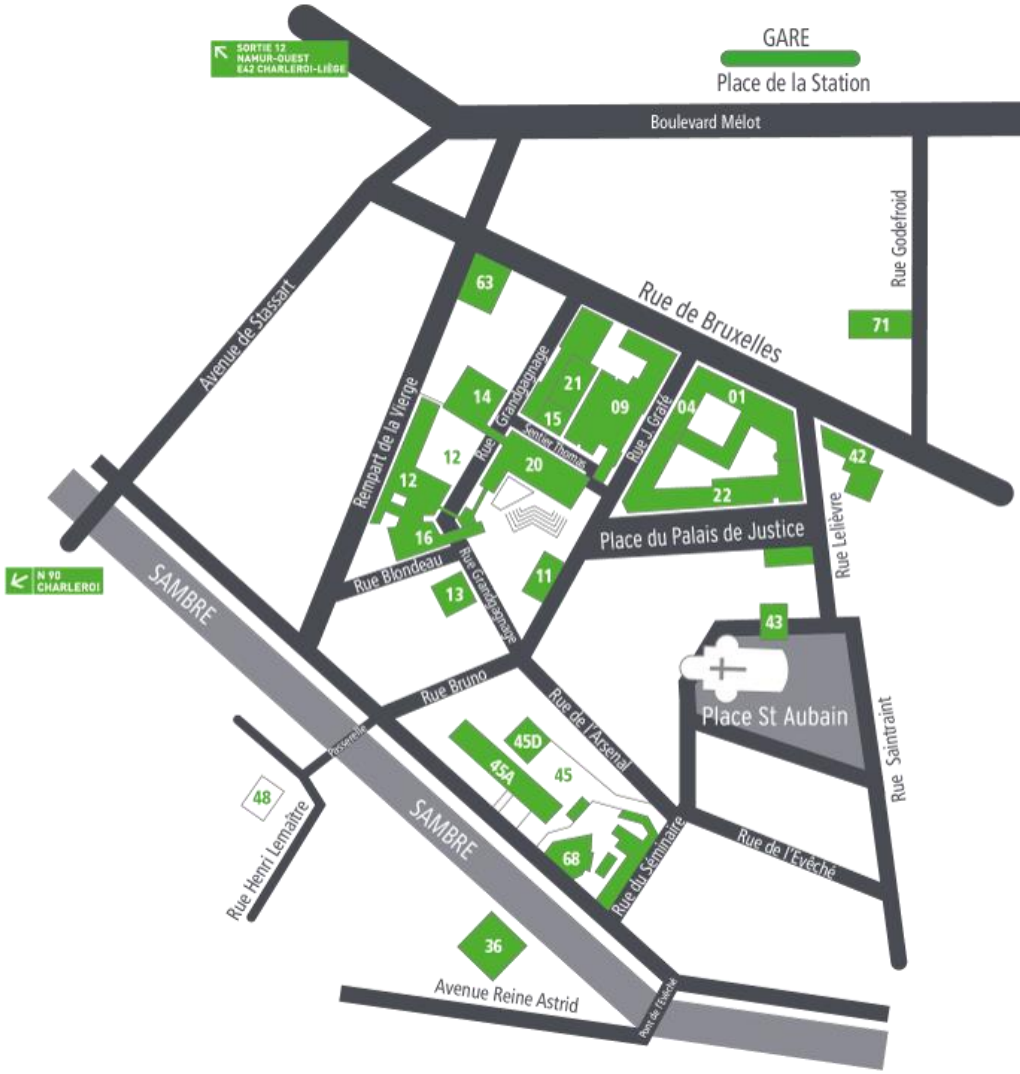

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