ETSF Newsletter

Winter Edition - March 2022

After being postponed for a year due to the pandemic, the informal ETSF workshop finally took place during December in Coimbra, Portugal.

For two days this was a much needed and welcomed opportunity for the community to meet and discuss in a relaxed environment about open topics in the field.
The first day was dedicated to new work on electron-phonon coupling (polarons, electron-phonon corrections, and Density Functional Perturbation Theory), quantum computing, and machine learning. On the second day the attendants had the chance to discuss topics related to spectroscopy (optical absorption of defects, trions), Green's functions methods (full frequency GW, finite momentum BSE, and real-time formalism) and their potential applications to optical detectors.

The fantastic environment allowed for several long discussions that prolonged late into the afternoon, risking in some cases attendance at the social events.
The social dinners were a great opportunity for attendants to laugh, enjoy the meal and continue the discussions they had during the day with a joyful approach.

Even in pandemic times, the local organisation team still managed to provide attendants with excellent venues for continued interaction that furthered discussions and networking. Certainly, all will be looking forward for the next opportunity to meet in such an informal fashion.

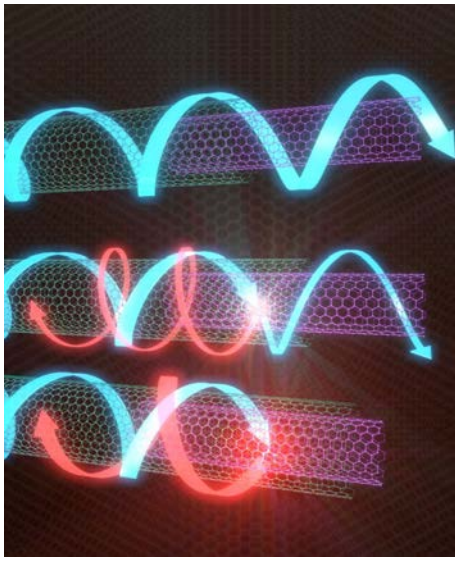
Focus Topic

Interference effects in one-dimensional moiré crystals

A study recently published in Carbon and led by Prof. ***Zeila Zanolli*** *from Utrecht University (The Netherlands) explores interlayer transport in one-dimensional moiré crystals as double-wall carbon nanotubes (DWNTs). The work provides a benchmark for experimental realizations of 1D moirés and correlated states in DWNTs. The results of this detailed study could be exploited to design quantum electronic devices, e.g. nanoelectronic switches based on chiral nanotubes.*

DWNTs, like twisted by layer graphene (tBLG), are a carbon-based moiré crystal, and examples of a tunable quantum material [1,2]. DWNTs possess two degrees of freedom controlling the emerging material properties: twist angle (like tBLG) and interlayer distance. While the physics emerging in 2D moiré crystals has been studied extensively, the understanding of its one-dimensional counterpart is limited to the ideal infinite nanotube case [3, 4, 5] and the commensurate, telescopic nanotubes [6, 7, 8, 9, 10, 11].

This work investigates interference effects in finite sections of 1D moiré crystals using the Landauer-Büttiker formalism within the tight-binding approximation. It explains interlayer transport in double-wall carbon nanotubes and demonstrates that wave function interference is visible at the mesoscale. Most importantly, the work sheds light on a 25-year-old mystery in quantum transport.
Measurements [12,13] found a conduction plateau of $1G_0$ in multiwall carbon nanotubes that cannot be explained as the simple addition of $2G_0$ contributions per conducting layer. The phenomenon remained unexplained until recently. The research team lead by Zeila Zanolli was finally able to demonstrate that the interlayer transmission in double-wall carbon nanotubes is limited to either $1G_0$ or $2G_0$, clarifying the origin of the $1G_0$ quantum conductance.



In addition, the researchers identified a class of nanotubes that show a behavior similar to a light switch. In practice, by moving the inner wall slightly in and out of the outer wall, it is possible to change between a conducting “on-state” and an non-conducting “off-state”. The discovery of switchable nanotubes opens up new avenues for the development of innovative nanoelectronics devices.

Reference article:
N. Wittemeier, M. J. Verstraete, P. Ordejón, Z. Zanolli, *Interference effects in one-dimensional moiré crystals*, Carbon **186**, 416 (2022) DOI: 10.1016/j.carbon.2021.10.028

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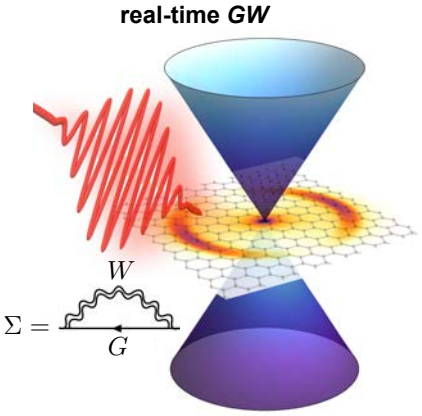
Scientific Highlights

Real-Time GW: Toward an *Ab Initio* Description of the Ultrafast Carrier and Exciton Dynamics in Two-Dimensional Materials – by E. Perfetto

The GW method, a popular tool to calculate electronic and optical properties of correlated ground states, is extended to the time domain to study ultrafast quantum phenomena in 2D materials. The great advantage of the proposed scheme is the linear scaling with the propagatation time, that renders the real-time GW method numerically competitive with TDDFT and Boltzmann Equation -based methods.



The performance of the appreach is explicitelty tested in two prototype 2D systems. In the case of photoexcited graphene it is found that the initial stage of the carrier multiplication process does not follow the typical exponential behavior predicted by the Markovian Boltzmann approach. For a resonantly pumped semiconductor a self-sustained screening cascade is discovered that produces the ultrafast melting of coherent excitons. These results draw attention to the importance of non-Markovian and dynamical screening effects in out-of-equilibrium phenomena.

Reference article:
E. Perfetto, Y. Pavlyukh, G. Stefanucci, Phys. Rev. Lett. 7;128(1):016801 (2022)
DOI: https://doi.org/10.1103/PhysRevLett.128.016801

Job Opportunities

Two post-doc positions in Milan:

● 24-months position funded by the FET project "SINFONIA" (https://www.sinfonia-fet.eu/) on ab initio calculation of electronic and optical properties of interfaces between organic molecules and anti-ferromagnetic surfaces to study the coupling of magnetic perturbation and optical stimuli in view of spintronic applications.

Deadline for application: 16/03/22 -- Starting: beginning of April
Contact person: guido.fratesi@unimi.it
Details at the dedicated UNIMI webpage

● 24-months position funded by NFFA (nnfa.eu) on ab initio characterization of local structure and stechiometry, electronic and magnetic properties of substitutional magnetic defects in 2D materials, as can be obtained via ultra-low energy implantation of magnetic atoms.

Deadline for application: 13/04/22 -- Starting: beginning of May
Contact person: simona.achilli@unimi.it
Details at the dedicated UNIMI webpage

Postdoc Positions at the Case Western Reserve University

CWRU has started a new program to attract high quality postdoctoral who would conduct research but also teach and get training in teaching and be mentored by current faculty(Presidential Society of STEM Post-Doctoral Fellows).

See https://case.edu/provost/presidential-fellows for more information.

1 PhD and 1 Post-Doc position in Germany

In coming 4 years jointly in Max Planck Inst. Halle and Max Born Inst. Berlin we will develop the Elk code to couple the nuclear degrees of freedom to the spin and charge dynamics in laser pumped systems treated using time-dependent density functional theory and to treat transient excitons in laser pumped 2D materials. This will be done by coupled time dependent density functional theory and Maxwell equations.
PhD program will last for 4 years and post-doc for 1+2 years.
Apply with CV, list of publications and contacts of 3 Referees writing to: sharma@mbi-berlin.de

Permanent position in the MSP team (IMEC):
Researcher in atomistic simulations for process modeling
For details see imec webpage (imec-int.com)

Upcoming Events

25th ETSF Workshop on Electronic Excitations: Fundamental challenges for theoretical spectroscopy from the frontier of technology to be held in Leuven, Belgium, from 13-17 June 2022

Registration is open! https://workshop.etsf.eu/

Deadline for *abstract submission* and *bursary applications*: **March 18th, 2022**

The 2022 edition of the workshop will include the traditional topics of interest of the ETSF community and focus on fundamental challenges for theoretical spectroscopy posed by cutting-edge present and future technologies, thereby promoting a fruitful exchange between academia and industry. The venue imec, an R&D hub for nano- and digital technologies, will serve as a gateway between industry and the academic world.

Topics covered by the workshop will include:

- Deep valence and upper core spectroscopy
- Time-resolved vibrational and electronic spectroscopy
- Dissipative quantum dynamics
- Photoresist radiation chemistry
- Multiscale and embedding methods
- Machine learning in theoretical spectroscopy

Introductory lectures:

- Geoffrey Pourtois, IMEC, Belgium
- Matthieu Verstraete, Université de Liège, Belgium

Invited speakers:

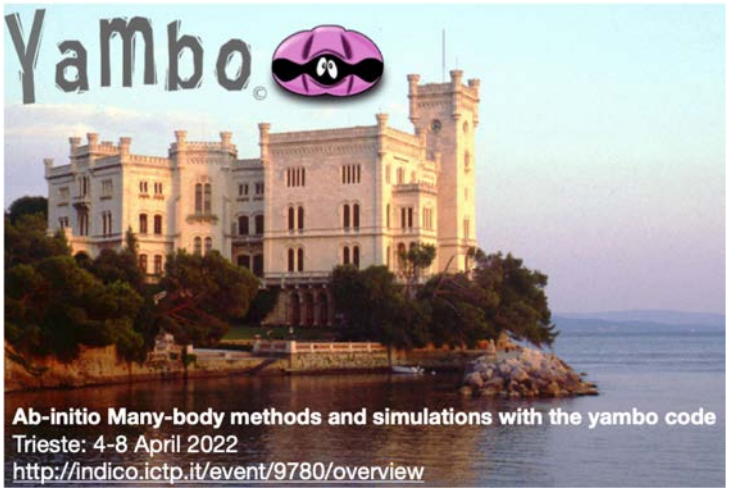
- Alex Chin, Sorbonne Université, France
- Dorothea Golze, TU Dresden, Germany
- Miquel Huix-Rotllant, Aix Marseille Université, France
- Milica Todorovic, University of Turku, Finland
- Mariana Rossi, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Francesco Sottile, École Polytechnique, France
- Nicolas Tancogne-Dejean, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
- Vladislav S. Yakovlev, Max Planck Institute of Quantum Optics, Germany
- Claudia Fleischman, IMEC and Katholieke Universiteit Leuven, Belgium
- Giulia Grancini, Università degli studi di Pavia, Pavia, Italy
- John Petersen, IMEC, Leuven, Belgium
- Eva Arianna Aurelia Pogna, CNR Nano, Pisa, Italy

⭐ **The Computational School on "Ab-initio Many-body Methods and Simulations with the Yambo Code"** will be held in Trieste from 4 to 8 April 2022.

The target participants are graduate students, postdocs, and researchers who are interested in learning or in improving their knowledge and skills to calculate electronic and optical properties of materials, beyond the well-known DFT limitations and using an efficient, highly parallelized and accurate many-body computational tool.

Both theoretical and technical lectures will be offered as well as dedicated hands-on sessions where students will learn how to use the code for materials of current research interest and how to optimize its use in a parallel environment. Several post-processing tools for the analysis of the results will be also introduced and practically applied. General topics will include self-energy and quasiparticles concepts, the GW approximation, and the Bethe-Salpeter equation, all placed in the context of and linked with experimental measurements (photoemission, absorption, photoluminescence).

At variance with previous editions, this school will present some advanced lectures such as: new algorithms developed to deal with electron-phonon interactions, real time evolution of equations of motion, time dependent polarization in terms of the Berry phase, and computation of non-linear optical properties. The specific usage in massively parallel environments equipped with modern accelerated video cards (GPU's) will be introduced. Due to the pandemic period the school is designed to allow participants to join part in person and part online.



A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.

Deadline
8th March 2022: in person participation
20th March 2022: remote participation

http://indico.ictp.it/event/9780/

Other relevant notes

Affiliation issue: we realized that ETSF affiliation is often not recognized in WOS.
We are looking into this and will complain to WOS - if you have the same experience or some insight into the problem please write to:
weissker@cinam.univ-mrs.fr , Matthieu.Verstraete@uliege.be, Francesco.Sottile@polytechnique.fr

To contribute to the Newsletter: write an email to simona.achilli@unimi.it