23rd ETSF Workshop on Electronic Excitations

Interdisciplinary Views on Quantum Many-Body Theory

Milan, Italy

10 – 14 September 2018

Welcome

The bi-annual workshop of the European Theoretical Spectroscopy Facility (ETSF) provides a forum for excited states and spectroscopy in condensed matter physics, chemistry, nanoscience, materials science, and molecular physics, attracting theoreticians, code developers, and experimentalists alike.

The 2018 edition aims at fostering the cross-fertilization between different approaches to many-body phenomena, transcending the traditional barriers between disciplines. The workshop will therefore bring together experts facing similar problems from different perspectives, for different applications, and often with a different language. Besides discussing application of many-body theories to excitations in condensed matter, i.e. the traditional field of expertise of ETSF, topics covered by the workshop will include nuclear physics, quantum chemistry, ultrafast excitation dynamics, quantum transport, topological insulators and novel algorithmic approaches to many-body problems inspired by machine learning and data science.

Workshop topics include:

- quantum chemistry
- nuclear physics
- machine learning / data science
- ultrafast excitation dynamics
- topological insulators
- quantum transport

We are glad to welcome you in Milan and wish you an inspiring workshop with lots of interesting science and fruitful discussions.

The organizers

General information

Organizing and program committee

- Giovanni Onida (University of Milan, Italy)
- Guido Fratesi (University of Milan, Italy)
- Zeila Zanolli (ICN2, Barcelona, Spain)
- Gabriele D'Avino (Institut Néel, CNRS, Grenoble, France)
- Michiel van Setten (IMEC, Leuven, Belgium)
- Claudia Rödl (Friedrich-Schiller-Universität Jena, Germany)

Local committee

- Giovanni Onida (University of Milan, Italy)
- Guido Fratesi (University of Milan, Italy)
- Simona Achilli (University of Milan, Italy)
- Elena Molteni (University of Milan, Italy)

ETSF steering committee

The ETSF steering committee (SC) consists of nine elected research team leaders (RTLs). The current SC members are:

- Matthieu Verstraete (Université de Liège, Belgium), Chair
- Claudio Attaccalite (Aix-Marseille Université, France)
- Arjan Berger (Université Paul Sabatier, Toulouse, France)
- Letizia Chiodo (Università Campus Bio-Medico di Roma, Rome, Italy)
- Rex Godby (University of York, UK)
- Myrta Grüning (Queen's University Belfast, UK)
- Gian-Marco Rignanese (Université Catholique Louvain-la-Neuve, Belgium)
- Francesco Sottile (Ecole Polytechnique, Palaiseau, France)
- Zeila Zanolli (ICN2, Barcelona, Spain)

Support

The organizers acknowledge financial support from the Ψ_k Network, the Young Academy of Europe, and the University of Milan.

Workshop venue

The workshop will be hosted by the **University of Milan** in the main hall of the **Faculty of Agricultural and Food Sciences**, close to the Physics Department and only 3 km from the very center of Milan (Duomo).

The **lecture room (room no. C03, at level -1)** can be accessed from **via Mangiagalli 25** (suggested) or from via Celoria 2. Another room (room no. C06) in the close proximity is available as workspace for the participants. Poster sessions and coffee breaks will be held just outside the mail hall.

Local contacts

Simona Achilli

Guido Fratesi

Elena Molteni

Internet access

Wi-fi is available in all Milan University areas via “eduroam”.

Posters

The poster boards will be situated just outside the main lecture hall. Posters can be put up starting from the early afternoon on Tuesday (11 September), the day of the poster session. Posters must be taken down by the coffee break on Friday morning (14 September).

Coffee breaks and lunch

There will be 30-min **coffee breaks** during morning (at 10:20) and afternoon (at 15:30) sessions. Coffee, tea, drinks, and snacks will be available just outside the conference room.

Lunch will be served at the **university canteen in via Clericetti** (see the map) upon presentation of the lunch ticket.

Conference desk

The conference desk will be located just at the entrance to the main lecture hall.

Social program

A **guided tour of the city center of Milan** will be organized after the scientific program on Thursday (13 September). Details about the meeting point and time will be provided during the workshop.

The **social dinner** will take place at the **restaurant “Serendipico”** in the city center **(piazza Castello 1, Subway MM1 - Cairoli)**. The dinner will start at 19:30. The transfer to/from the restaurant will be organized by public transport (see below).

People interested in these events will be asked to confirm their participation during the meeting where further schedule details will be provided.

Transportation

The conference location, the canteen for lunches, suggested hotels, and some suggested restaurants (not endorsed by the organization) are within walking distance from each other in the “Città Studi” district. **Public transport** in the district, to reach the city center, or main train stations is served by ATM company. **Bike sharing** is also very popular in the area.

To reach the **railway stations Milano Centrale, Milano Porta Garibaldi, Milano Nord Cadorna**, take the subway line M2 (green line) at Piola, direction Abbiategrasso or Assago Forum, stop at Centrale, Garibaldi, Cadorna respectively.

To reach the **city center**, take subway line M2 (green line) at Piola towards Abbiategrasso or Assago Forum, stop at Loreto. There, take line M1 (red line) towards Rho or Bisceglie, stop at Duomo or nearby stops.

A **schedule explorer** is available at www.atm-mi.it (info on subway, tram, and bus lines). Smartphone apps like Moovit are also typically helpful and reliable in town.

To reach **Milano Malpensa** airport, a train service is available (www.trenitalia.com). **Milano Linate** is served by ATM urban bus no. 73 passing close by the university. **Bergamo** airport is best reached by shuttle buses from Milano Centrale. Shuttle buses also serve the other two airports.

Information about reaching the welcome drink place, the meeting point of the walking tour, and the social dinner will be provided during the conference.

Program

	Monday, 10 September: Registration and introductory lectures
14:00	Steering committee meeting
15:30	Registration & coffee
16:00	Opening
16:10	Hardy Gross – Ab-initio prediction of quantum phases and their dynamics far from equilibrium
16:50	Stefano Carrazza – Advanced machine learning approaches
19:00	Welcome drink

	Tuesday, 11 September: GW and nuclear physics
09:00	Patrick Rinke – *GW* and beyond: core excitations, strong correlation and artificial intelligence
09:40	Christian Vorwerk – X-ray Absorption and Scattering Spectroscopy in Solids from Many-Body Perturbation Theory
10:00	Brian Cunningham – Ladder diagrams in the Quasiparticle self-consistent GW method
10:20	Coffee break
10:50	Rex Godby – *GW*-type approximations and TDDFT response functions using exactly solvable real-space model systems
11:10	ETSF general meeting
11:55	ETSF website presentation
12:10	Lunch
14:10	Gianluca Colò – Density Functional Theory (DFT) concepts and implementations in nuclear physics
14:50	Valerio Olevano – Condensed-matter and nuclear physics many-body approaches compared to the helium atom exact solution
15:10	Christoph Friedrich – Electron-magnon scattering in elementary ferromagnets from first principles: lifetime broadening and kinks
15:30	Samuel Poncé – Predictive calculations of phonon-limited carrier mobilities in semiconductors
15:50	Alberto Castro – Propagators for the non-linear time-dependent equations in quantum many-body theory
16:10	Poster session (food & drinks)

	Wednesday, 12 September: Ultrafast phenomena and topological insulators
09:00	Giulio Cerullo – Ultrafast carrier and spin dynamics in two-dimensional semiconductors
09:40	Pedro Melo – Non-equilibrium real-time dynamics on TMDs: photoluminescence and Kerr signals
10:00	Florian Eich – Time-dependent charge and energy transport in nanoscale devices
10:20	Coffee break
10:50	Irene Burghardt – Ultrafast Vibronic Dynamics of Functional Organic Polymer Materials: Coherence, Confinement, and Disorder
11:30	Claudio Verdozzi – KBE, GKBA, and Ehrenfest Dynamics
11:50	Tuomas Rossi – Real-time TDDFT modeling of localized surface plasmon formation and decay into hot carriers
12:10	Lunch
14:10	Cristiane de Morais-Smith – There is plenty of room at the bottom, but even more in a fractal
14:50	Matteo Cococcioni – First-principles modeling of mixed-valence compounds from extended Hubbard-corrected functionals
15:10	Nicolas Tancogne-Dejean – Ultrafast modification of Hubbard U in a strongly correlated material: *ab initio* high-harmonic generation in NiO
15:30	Coffee break
16:00	Markus Morgenstern – Giant tuning of graphene's pseudospin polarization and valley splitting by a scanning tunneling microscope
16:40	Davide Grassano – Validity of Weyl fermion picture for transition metals monopnictides TaAs, TaP, NbAs, and NbP from ab initio studies
17:00	Science policy (round table)
	Luisa Torsi – The role of women in science: still a long way to go
	Tomas Brage – Why is physics still so gendered - and what can we do about it?

	Thursday, 13 September: Data science and quantum chemistry
09:00	Miguel Marques – Applications of machine learning to materials science
09:40	Michiel van Setten – Predicting alloy properties, machine learning the gap between experiment and ab initio
10:00	Pedro Borlido – Structural prediction of free-standing 2-D materials
10:20	Coffee break
10:50	Matthieu Verstraete – From one to three, exploring the rungs of Jacob's ladder in magnetic alloys
11:10	Gabriele D'Avino – Electronic excitations in molecular solids from embedded many-body perturbation theory: fundamentals and applications
11:30	Giulia Galli – Computational spectroscopy at finite temperature
12:10	Lunch
14:10	Petra Rudolf – Free surfaces recast superconductivity in few monolayer MgB2: Combined first-principles and ARPES demonstration
14:50	Zeila Zanolli – DFT & electron holography
15:10	Ludger Wirtz – New developments for resonant Raman scattering and phonon-assisted indirect absorption/emission
15:30	Pierluigi Cudazzo – Cumulant expansion of the electronic polarizability: beyond the static Bethe-Salpeter equation
15:50	Claudio Attaccalite – Invisible excitations in hexagonal Boron Nitride
16:10	Social program
19:30	Workshop dinner

	Friday, 14 September: Quantum chemistry and transport
09:00	Cristiana Di Valentin – Quantum Chemical Simulations of Stimuli–Responsive Nanomaterials for Biomedical Applications
09:40	Alberto Milani – End-group effects in tuning the semiconductor-to-metal transition of carbon atom wires: insights from first-principles calculations
10:00	Anu Baby – Impact of alkali metal-doping on the electronic and optical properties of organic molecules adsorbed on metal surface
10:20	Coffee break
10:50	Rocco Martinazzo – Why Silicon is not Carbon?
11:30	Simona Achilli – GeV$_n$ defects in silicon: a viable route toward high temperature single electron transport
11:50	Nicole Helbig – Nonadiabatic Dynamics in Single-Electron Tunneling Devices with Time-Dependent Density-Functional Theory
12:10	Davide Sangalli – An ab-initio approach to describe coherent and non-coherent exciton dynamics
12:30	Closing remarks
12:45	Lunch

Oral contributions

Ab-initio prediction of quantum phases and their dynamics far from equilibrium

E.K.U. Gross

Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

The basic idea of “functional theories” is to describe nature in terms of a simple, reduced quantity rather than the full many-body wave function. Prominent examples of functional theories are density-functional theory as well as Green-function-functional theory (better known as many-body perturbation theory). After an overview of the basic concepts of standard ground-state density functional theory (DFT) as well as time-dependent DFT (TDDFT), and their relation to Green-function-functional theory, the description of quantum phases, such as magnetism and superconductivity within these frameworks will be addressed. The idea is to include the order parameter describing the respective quantum phases or the corresponding propagator explicitly [1,2] in the formalism as an additional density or an additional Green’s function. This can be done both in the static case and in systems driven far from equilibrium. As a real-world example, the laser-induced demagnetization of ferromagnets [3] and the ultrafast spin transfer between magnetic sublattices [4] will be calculated by real-time TDDFT. Furthermore, some thoughts will be presented [5] on how to tackle systems containing more than one type of particles, such as electrons and nuclei, if they fully interact beyond the Born-Oppenheimer approximation. As a particular manifestation of Beyond-Born-Oppenheimer dynamics, the molecular Berry phase will be discussed [6].

[1] O.J. Wacker, R. Kuemmel, E.K.U. Gross, Phys. Rev. Lett. 73, 2915 (1994)
[2] F.G. Eich, E.K.U. Gross, Phys. Rev. Lett. 111, 156401 (2013)
[3] K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma, E.K.U. Gross, JCTC 11, 4870 (2015)
[4] J.K. Dewhurst, P. Elliott, S. Shallcross, E.K.U. Gross, S. Sharma , Nano Lett. 18,1842 (2018)
[5] A. Abedi, N.T. Maitra, E.K.U. Gross, Phys. Rev. Lett. 105, 123002 (2010)
[6] S.K. Min, A. Abedi, K.S. Kim, E.K.U. Gross, Phys. Rev. Lett. 113, 263004 (2014)

Advanced machine learning approaches

S. Carrazza

Theoretical Physics Department, CERN, CH-1211 Geneva 23, Switzerland

We provide an introduction to machine learning concepts and methods supported by examples in computer science and physics. We then provide a discussion about its implications for natural science highlighting the current advantages, implementation challenges and future directions. Finally, we conclude the discussion by showing an example about the construction of new machine learning architectures and algorithms based on the interpretation of statistical physics systems.

GW and beyond: core excitations, strong correlation and artificial intelligence

Patrick Rinke

Aalto University, School of Science, 00076 Aalto, Finland

The GW approximation to many-body perturbation theory (MBPT) has been incredibly successful in theoretical spectroscopy. Yet, challenges abound and new frontiers await. In this presentation, I will introduce our first exploration of perturbative GW (G_0W_0) for core excitations [1]. We have implemented the real-frequency contour deformation technique into the all-electron numerical atomic orbital code FHI-aims [2]. The real-frequency treatment proves to be necessary to treat core excitations accurately. The computed core level binding energies deviate by generally less than 0.5 eV from experiment (on an absolute scale) outperforming the popular density-functional theory based Delta Self-Consistent Field (ΔSCF) method. To tackle strongly correlated systems, we have developed a new quantum embedding theory [3]. It captures strong (static) correlation in a subspace by configuration interaction (CI) theory and high-energy dynamic correlation with MBPT in the GW and Bethe-Salpeter equation (BSE) approximation. For the challenging multi-reference problems of H_2 and N_2 dissociation, we obtain good agreement with benchmark results. Our theory treats ground and excited states on equal footing, and we compute vertical excitation energies of N_2 and free-base porphyrin in excellent agreement with high level quantum chemistry methods. Despite the successes of theoretical spectroscopy, spectroscopic calculations and experiments are (computationally) expensive. For this reason, we recently investigated artificial intelligence (AI) enhanced spectroscopy that can learn from the plethora of already available experimental and theoretical spectroscopy data. Once trained, the AI can make predictions of spectra instantly and at no further cost. I will present artificial neural networks that can learn excitation spectra of molecules [4].

*This work was performed in collaboration with A. Stuke, K. Ghosh, L. Himanen, M. Todorović, and A. Vehtari

[1] D. Golze, J. Wilhelm, M. van Setten, and P. Rinke, Core level binding energies from *GW*: An efficient full-frequency approach within a localized basis, under review
[2] X. Ren, P. Rinke *et al.*, Resolution-of-identity approach to Hartree-Fock, hybrid density functionals, RPA, MP2, and *GW* with numeric atom-centered orbital basis functions, New J. Phys. **14**, 053020 (2012)
[3] M. Dvorak, D. Golze, and P. Rinke, A quantum embedding theory combining configuration interaction with *GW*/BSE, under review
[4] K. Ghosh, A. Stuke, M. Todorović, P. B. Jørgensen, M. N. Schmidt, A. Vehtari, and P. Rinke, Deep learning spectroscopy: neural networks for molecular excitation spectra, under review

X-ray Absorption and Scattering Spectroscopy in Solids from Many-Body Perturbation Theory

Christian Vorwerk[1,2], Caterina Cocchi[1,2], and Claudia Draxl[1,2]

[1] *Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany*
[2] *European Theoretical Spectroscopy Facility*

X-ray absorption and inelastic scattering spectroscopy are powerful tools to investigate the local electronic and structural properties of crystalline materials. The accurate determination of these spectra from first principles requires a reliable description of the electron-core hole interaction, which is typically screened by the surrounding many-electron system. We present an approach to core excitations through the solution of the Bethe-Salpeter equation (BSE), including the full non-local screened interaction between electron and core hole. Our implementation in the `exciting` [1] package makes use of highly precise Kohn-Sham single-particle energies and wavefunctions for both the core and conduction region. These wavefunctions are obtained on equal footing from all-electron full-potential DFT calculations. Here, we discuss the effects of many-body interactions on the core spectra of oxide materials, ranging from CaO [2], to the wide-gap transparent oxide Ga_2O_3. We reveal fingerprints of the local electronic structure surrounding the absorbing atoms, and analyze the influence of correlation effects on the spectra.

[1] A. Gulans *et al.*, *J. Phys. Condens. Matter* **26**, 363202 (2014).
[2] C. Vorwerk, C. Cocchi, and C. Draxl, *Phys. Rev. B* **95**, 155121 (2017).

Ladder diagrams in the Quasiparticle self-consistent GW method

B. Cunningham[1], M. Grüning[1], and M. van Schilfgaarde[2]

[1] *Atomistic Simulation Centre, Queen's University Belfast, University Road, Belfast BT71NN, UK*
[2] *Theory & Simulation of Condensed Matter, King's College London, Strand, London WC2R 2LS, UK*

The accurate description of electrons in solids is essential for advances in science, computing and technology. Methods that go beyond the widely used Density Functional Theory (DFT) and its extension are required for many systems of interest. QSGW [1] is a method that optimizes the GW approximation of Hedin's equations, and removes the DFT dependence. QSGW is an accurate method that can be applied to many systems where DFT and DFT-based GW (i.e., G_0W_0) ultimately fail.

The neglection of vertex contributions in the QSGW polarization, however, leads to a (sometimes rather large) systematic band gap overestimation. In this work we include vertex contributions by solving the Bethe-Salpeter equation for the full polarization matrix at all **k**-vectors in the Brillouin zone and use this to include ladder diagrams in the QSGW self-energy. Vertex contributions corrects – to a large extent – the band gap overestimation and produces a better estimate for the static dielectric constant.

These methods were implemented in the full potential community package Questaal [2]; part of the CCP flagship project: Quasiparticle Self-Consistent GW for Next-Generation Electronic Structure [3]. Implementation of vertex contributions in W are discussed and results for the electronic structure and optical absorption spectra [4] are presented.

[1] T. Kotani et al., Phys. Rev. B **76**, 165106 (2007)
[2] https://www.questaal.org
[3] https://www.ccp9.ac.uk/QSGWflagship [4] Cunningham et al., Phys. Rev. Mat. **2**, 034603 (2018)

Assessing *GW*-type approximations and TDDFT response functions using exactly solvable real-space model systems

Jack Wetherell[1,2], Mike Entwistle[1,2], Leopold Talirz[1,2,3], Matt Hodgson[4,2], and Rex Godby[1,2]

[1] *Department of Physics, University of York, York YO10 5DD, United Kingdom*
[2] *European Theoretical Spectroscopy Facility*
[3] *EPFL Valais Wallis, CH-1951 Sion, Switzerland*
[4] *Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany*

We investigate approximations related to the one- and two-particle Green's functions for many-electron systems, using new functionality of the iDEA code [1] in which the many-electron Schrödinger equation is solved exactly for simple one-dimensional model systems. First, we assess the accuracy of a comprehensive set of GW-like approximations for calculating the one-particle Green's function, in particular quasiparticle energies and electron densities [2]. The methods assessed include fully self-consistent, partially self-consistent and non-self-consistent (from different starting points) GW, plus approximations based on static screening of the Coulomb interaction. A simple vertex correction to compensate for self-screening [3] is also presented. Second, we turn to an important aspect of the two-particle Green's function, the density-response function χ, including the optical absorption spectrum, with a focus on the prospects for improving the description of χ in time-dependent DFT. The key step in this process, the dynamic exchange-correlation kernel $f_{\mathrm{xc}}(x, x', \omega)$, is studied by first calculating the exact response function χ for the interacting system, and its counterpart for the auxiliary system of non-interacting electrons of exact Kohn-Sham DFT, χ_{KS} [4].

[1] http://www-users.york.ac.uk/ rwg3/idea.html
[2] J. Wetherell, L. Talirz, M.J.P. Hodgson and R.W. Godby, unpublished
[3] "GW self-screening error and its correction using a local density functional", J. Wetherell, M.J.P. Hodgson and R.W. Godby, Physical Review B (Rapid Communications) **97** 121102(R) (2018)
[4] M.T. Entwistle and R.W. Godby, unpublished

Density Functional Theory (DFT) concepts and implementations in nuclear physics

G. Colò

Dipartimento di Fisica, Università degli Studi, and INFN Sez. di Milano, via Celoria 16, 20133 Milano, Italy

The nuclear many-body problem has many similarities with the electronic many-body problem, as recognised already long ago. I will first give a brief survey of the status of nuclear structure theory, and emphasize the role of Density Functional Theory (DFT) as the framework in which the mutual cross-fertilization between nuclear physics and physics of matter, or chemistry, may work at best. I will discuss some applications of the most recent DFT-based theoretical models to the global ground-state properties of nuclei. Then, I will single out a few specific aspects. I will discuss collective nuclear excitations, or giant resonances, as well as their importance to deduce from the experiment the so-called nuclear equation of state (EoS), that is, the relationship between pressure and density in nuclear matter. This connects nuclear physics and the physics of a gas or a liquid. It also allows to set a link with the macroscopic scale of those "nuclei" that have dimensions of km, namely neutron stars. I will also discuss the low-lying nuclear spectra, that play an important role to identify relevant nuclear correlations like those related to the coupling between single-particle motion and the vibrations or rotations of the nucleus as a whole. The limitations of current EDFs and the theories that resemble the electronic GW, although having different names, will be mentioned. Finally, if time allows, I will briefly touch upon the inverse Kohn-Sham problem in nuclear physics.

Condensed-matter and nuclear physics many-body approaches compared to the helium atom exact solution

V. Olevano

CNRS, Institut Néel Université de Grenoble-Alpes

The helium atom is a lucky and unique many-body system (though only two-body) in which, thanks to the 1929 pioneering work of Hylleraas, we own an exact solution (today up to 40 digits octuple precision) of the Schrödinger equation. Moreover, it is even a real system. Here we use it as a benchmark for comparison between many-body methods coming from condensed matter, nuclear physics and quantum chemistry. We will compare the exact Hylleraas solution to full configuration interaction (CI), quantum Monte Carlo (QMC, both variational VMC and diffusion DMC), density-functional theory (DFT) and time-dependent DFT (TDDFT), direct RPA and full RPA with exchange (aka time-dependent Hartree-Fock, TDHF), Bethe-Salpeter equation (BSE) on top of GW, and finally a renormalized RPA (r-RPA) in the framework of the self-consistent RPA (SCRPA) originally developed in nuclear physics.

Electron-magnon scattering in elementary ferromagnets from first principles: lifetime broadening and kinks

C. Friedrich, M. C. T. D. Müller, and S. Blügel

Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

We study the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory implemented in the full-potential linearized augmented-plane-wave method. To this end, a **k**-dependent self-energy describing the scattering of electrons and magnons is constructed from the solution of a Bethe-Salpeter equation for the two-particle (electron-hole) Green function, in which single-particle Stoner and collective spin-wave excitations (magnons) are treated on the same footing. Partial self-consistency is achieved by the alignment of the chemical potentials. The resulting renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. The renormalization gives rise to kinks in the electronic band dispersion at low binding energies, which we attribute to electron scattering with spatially extended spin waves. Furthermore, we find a band anomaly at larger binding energies in iron, which results from a coupling of the quasihole with single-particle excitations that form a peak in the Stoner continuum.

Predictive calculations of phonon-limited carrier mobilities in semiconductors

S. Poncé[1], E. R. Margine[2], and F. Giustino[1,3]

[1] *Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom*
[2] *Department of Physics, Binghamton University-SUNY, Binghamton, New York 13902, USA*
[3] *Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA*

The ability to predictively and reliably compute electron-phonon coupling properties for periodic solids within DFT was only recently developed using frozen-phonon methods [1] or density functional perturbation theory [2,3].
In this talk, we will probe the accuracy limit of *ab initio* calculations of carrier mobilities that relies on the electron-phonon coupling, within the framework of the Boltzmann transport equation [4]. In particular, we will show that predictive calculations of electron and hole mobilities require many-body quasiparticle corrections to band structures and electron-phonon matrix elements, the inclusion of spin-orbit coupling, and an extremely fine sampling of inelastic scattering processes in momentum space [5].
Such fine sampling calculation is made possible at an affordable computational cost through the use of efficient Fourier-Wannier interpolation of the electron-phonon matrix elements as implemented in the EPW code [6].
We will discuss recent findings on the mobility of silicon, wurtzite GaN and halide perovskites.

[1] C. E. Patrick and F. Giustino, Nat. Commun. **4**, 2006 (2013).
[2] F. Giustino, S. G. Louie, and M. L. Cohen, Phys. Rev. Lett. **105**, 265501 (2010).
[3] G. Antonius, S. Poncé, P. Boulanger, M. Côté, and X. Gonze, Phys. Rev. Lett. **112**, 215501 (2014).
[4] J. Ziman 1960; G. Grimvall 1981; G. D. Mahan 2000.
[5] S. Poncé, E. R. Margine and F. Giustino, Phys. Rev. B **97**, 121201 (2018).
[6] S. Poncé, E. R. Margine, C. Verdi, and F. Giustino, Comput. Phys. Commun. **209**, 116 (2016).

Propagators for the non-linear time-dependent equations in quantum many-body theory

Adrián Gómez Pueyo[1], Miguel A. L. Marques[2], Angel Rubio[3,4,5], and Alberto Castro[6,1]

[1] *Institute for Biocomputation and Physics of Complex Systems, University of Zaragoza, Calle Mariano Esquillor, 50018 Zaragoza, Spain*
[2] *Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany*
[3] *Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany*
[4] *Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York, New York 10010, United States*
[5] *Nano-Bio Spectroscopy Group, Universidad del País Vasco, 20018 San Sebastián, Spain*
[6] *ARAID Foundation, Avenida de Ranillas 1, 50018 Zaragoza, Spain*

We examine various integration schemes valid for the non-linear equations that emerge in general in any formulation of a time-dependent quantum many-body problem. We have focused in particular in the Kohn–Sham equations of time-dependent density-functional theory. Contrary to the time-dependent Schrödinger's equation, this set of equations is nonlinear, due to the dependence of the Hamiltonian on the electronic density. We discuss some of their exact properties, and in particular their symplectic structure. Four different families of propagators are considered, specifically the linear multistep, Runge-Kutta, exponential Runge-Kutta, and the commutator-free Magnus schemes. These have been chosen because they have been largely ignored in the past for time-dependent electronic structure calculations. The performance is analyzed in terms of cost-versus-accuracy. The clear winner, in terms of robustness, simplicity, and efficiency is a simplified version of a fourth-order commutator-free Magnus integrator. However, in some specific cases, other propagators, such as some implicit versions of the multistep methods, may be useful.

[1] A. Gómez Pueyo, M. A. L. Marques, A. Rubio, and A. Castro, J. Chem. Theor. Comp. 14, 3040 (2018). DOI: 10.1021/acs.jctc.8b00197

Ultrafast carrier and spin dynamics in two-dimensional semiconductors

Giulio Cerullo

Dipartimento di Fisica, Politecnico di Milano, Italy

In layered semiconductors, such as transition metal dichalcogenides (TMD), the electron-electron interaction is strongly enhanced by both quantum confinement and reduced screening. Furthermore, in these materials the valley polarization can be optically controlled by means of circularly polarized light. Here we discuss the ultrafast optical response of TMDs, focusing on two aspects: time-resolved measurements of exciton dynamics and spin/valley relaxation processes. We first study exciton dynamics in single-layer (1L) MoS2 by broadband femtosecond transient absorption spectroscopy combined with time-resolved ab-initio simulations based on the non-equilibrium Green's functions and density-functional theory. This comparison indicates that the non-equilibrium optical properties of TMDs are influenced by the renormalisation of both band gap and exciton binding energies caused by photo-excited charge carriers. We further use sub-20-fs pump pulses tuned above the electronic gap to study the exciton formation process in 1L-MoS2, and determine a build-up time of 35 fs. This is consistent with a scenario where free carriers, initially excited above the quasi-particle gap, relax towards lower energy states and finally form the exciton state via the strong Coulomb interaction. The exciton valley relaxation dynamics is investigated by time-resolved Faraday rotation. We observe a double exponential decay, with an initial fast (200fs) decay due to scattering of spin-polarized excitons from K to K'. This is in good agreement with the time scale predicted by the Maialle-Silva-Sham electron/hole exchange interaction mechanism, which can be interpreted as a virtual annihilation of a bright exciton in one valley followed by the creation of an exciton in the opposite valley. Finally, use two-colour helicity-resolved pump-probe spectroscopy in order to disentangle the intervalley and intravalley spin-flip processes of electrons in the conduction band of 1L-WS2. Spin-polarized carriers are injected by a circularly polarized pump pulse resonant with the A exciton, while the co-circularly polarized probe pulse is tuned around the B excitonic peak. In this configuration, the scattering of the electrons from the upper to the lower conduction band level (where they cannot radiatively recombine) is detected by measuring the build-up dynamics of the bleaching signal around the B exciton caused by Pauli blocking. We also show that spin-conserving intervalley scattering dynamics occur on a faster time-scale than the intraband spin-flip process.

Non-equilibrium real-time dynamics on TMDs: photoluminescence and Kerr signals

Pedro Melo[1,2], Andrea Marini[3,2], Matthieu Verstraete[1,2], and Zeila Zanoli[4,2]

[1] *Nanomat lab, Q-Mat center, CESAM Research Unit, Universite de Liège, Institut de Physique, Bat. B5a, 3/7, Allée du 6 aout, 19 B-4000 Sart Tilman, Liège, Belgium*
[2] *European Theoretical Spectroscopy Facility*
[3] *Consiglio Nazionale delle Ricerche (CNR),Via Salaria Km 29.3, CP 10, 00016, Monterotondo Stazione, Italy*
[4] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), Campus Bellaterra, 08193 Barcelona, Spain*

The interest in properties of transition metal dichalcogenides (TMDs) has increased due to the discovery of the coupling between spin and valley degrees of freedom and bright photoluminescence (PL). The theoretical study of the latter has been hindered due to lack of predictive ab initio numerical techniques [1,2,4]. We present a complete theoretical framework for the computation of PL where electrons, nuclei, and photons are quantised. The intrinsic non-equilibrium nature of the process is fully taken into account [3]. Starting from the Keldysh contour, we arrive at a set of equations for the Green's functions of electrons, phonons, and photons. These equations are then simplified by using the generalised Baym-Kadanoff ansatz and the completed collision approximation [3]. This reduces the problem to a set of decoupled equations for the density matrix that describe all kinds of static and dynamical correlations. We show how the micro-macro connection relates the observable spectrum with the time-dependent microscopic dynamics, via the Bethe-Salpeter equation. Finally, we present the results of our numerical studies on 2D TMDs, where we relate the evolution of the carrier populations due to electron-phonon interaction in the Brillouin zone with the changes in the PL spectrum and Kerr rotation signals of the materials.

[1] M. F. Pereira and K. Henneberger, Phys. Rev. B 58, 2064 (1998).
[2] K. Hannewald, et al, Phys. Rev. B 67, 233202 (2003).
[3] P. M. M. C. de Melo and A. Marini, Phys. Rev. B 93, 155102 (2016).
[4] S. W. Koch, et al, Nat Mat 5, 523 (2006).

Time-dependent charge and energy transport in nanoscale devices

F. G. Eich

Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg, Germany

Thanks to recent advances in ultra-fast pump-probe spectroscopies and nano-thermometry it is possible to study charge and energy flow at atomic time and length scales. In order to analyze the transient dynamics of nanoscale devices theoretically, nonequilibrium thermal Density-Functional Theory [1,2] provides a novel framework to address charge and energy currents on the same footing. In my talk I present our recent investigation of the applicability of the wide-band limit to the study of charge and heat transport through nanojunctions exposed to voltage biases and temperature gradients [3]. Moreover, I discuss our recent efforts to implement a numerically efficient propagation scheme capable to simulate mesoscopic transport devices.

[1] F. G. Eich, M. Di Ventra, and G. Vignale, Phys. Rev. Lett. **112**, 196401 (2014)
[2] F. G. Eich, M. Di Ventra, and G. Vignale, J. Phys.: Condens. Matter **29** 063001 (2017)
[3] F. Covito, F. G. Eich, R. Tuovinen, M. A. Sentef, and A. Rubio, J. Chem. Theory Comput., **14** (5), 2495 (2018)

Ultrafast Vibronic Dynamics of Functional Organic Polymer Materials: Coherence, Confinement, and Disorder

I. Burghardt

Goethe University Frankfurt, Institute of Physical and Theoretical Chemistry, Max-von-Laue-Str. 7, 60438 Frankfurt, Germany

This talk addresses quantum dynamical studies of ultrafast photo-induced energy and charge transfer in functional organic materials, complementing time-resolved spectroscopic observations [1] which underscore that the elementary transfer events in these molecular aggregate systems can be guided by quantum coherence, despite the presence of static and dynamic disorder. The intricate interplay of electronic delocalization, coherent vibronic dynamics, and trapping phenomena requires a quantum dynamical treatment that goes beyond conventional mixed quantum-classical simulations. Our approach combines first-principles parametrized Hamiltonians [2], based on TDDFT and/or high-level electronic structure calculations, with accurate quantum dynamics simulations using the Multi-Configuration Time-Dependent Hartree (MCTDH) method [3] and its multi-layer (ML-MCTDH) variant [4], along with semiclassical methods [5]. The talk will specifically focus on (i) exciton dissociation and free carrier generation in regioregular donor-acceptor assemblies [2,6], and (ii) the elementary mechanism of exciton migration and creation of charge-transfer excitons in polythiophene and poly-(p-phenylene vinylene) type materials [5,7]. Special emphasis is placed on the influence of structural (dis)order and molecular packing, which can act as a determining factor in transfer efficiencies. Against this background, we will comment on the role of temporal and spatial coherence along with a consistent description of the transition to a classical-statistical regime.

[1] A. De Sio and C. Lienau, Phys. Chem. Chem. Phys. **19**, 18813 (2017).
[2] M. Polkehn, P. Eisenbrandt, H. Tamura, and I. Burghardt, Int. J. Quantum Chem. **118**:e25502. (2018).
[3] G. A. Worth, H.-D. Meyer, H. Köppel, L. S. Cederbaum, and I. Burghardt, Int. Rev. Phys. Chem. **27**, 569 (2008).
[4] H. Wang, J. Phys. Chem. A **119**, 7951 (2015).
[5] R. Liang, S. J. Cotton, R. Binder, I. Burghardt, and W. H. Miller, J. Chem. Phys. **149**, 044101 (2018).
[6] M. Polkehn, H. Tamura, and I. Burghardt, J. Phys. B: At. Mol. Opt. Phys. **51**, 014003 (2018).
[7] R. Binder, D. Lauvergnat, and I. Burghardt, Phys. Rev. Lett., **120**, 227401 (2018).

KBE, GKBA, and Ehrenfest Dynamics

E. Boström[1,2], M. Hopian[1,2], P. Helmer[1], A. Mikkelsen[1], E. Perfetto[3,4,2], G. Stefanucci[4,5,2], P. Werner[6], and C. Verdozzi[1,2]

[1] *Lund University, Department of Physics, PO Box 118, 22100 Lund, Sweden*
[2] *European Theoretical Spectroscopy Facility*
[3] *CNR-ISM, Division of Ultrafast Processes in Materials (FLASHit)*
[4] *INFN, Sezione di Roma Tor Vergata, Via della Ricerca Scientica 1, 00133 Roma, Italy*
[5] *Dipartimento di Fisica,Universita di Roma Tor Vergata, Via della Ricerca Scientica 1, 00133 Rome, Italy*
[6] *Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland*

We use NEGF in the Generalized-Kadanoff-Baym approximation in conjunction with the Ehrenfest dynamics for nuclei to study the dynamical role of electronic correlations in i) donor-acceptor complexes, and ii) quantum transport geometries (i.e. dynamical friction in molecular motors). A discussion of work in progress related to this topic is also provided.

Real-time TDDFT modeling of localized surface plasmon formation and decay into hot carriers

T. P. Rossi[1], P. Erhart[1], and M. Kuisma[2]

[1] *Department of Physics, Chalmers University of Technology, Gothenburg, Sweden*
[2] *Department of Chemistry, University of Jyväskylä, Jyväskylä, Finland*

Localized surface plasmons render metal nanoparticles efficient light absorbers at their resonance frequencies. After its excitation, the plasmon resonance decays into high-energy electrons and holes, which, combined with the large absorption cross section, makes metal nanoparticles attractive hot-carrier generators for photocatalysis. In this work, we study the femtosecond real-time dynamics of localized surface plasmons in noble metal nanoparticles by using time-dependent density-functional theory (TDDFT). By extending the frequency-space Kohn–Sham decomposition analysis [1] to real time, we follow the plasmon formation as a collective excitation, track its subsequent decay into incoherent electron-hole transitions, and finally, obtain the corresponding hot-carrier distributions. Our work paves the way for addressing the spatiotemporal dynamics of hot-carrier generation in catalytically-relevant edge and corner sites of nanoparticles.

[1] T. P. Rossi et al., J. Chem. Theory Comput. **13**, 4779 (2017).

There is plenty of room at the bottom, but even more in a fractal

S. N. Kempkes[1] . M. R. Slot[2], S. E. Freeney[2], S. J. M. Zevenhuizen[2], D. Vanmaekelbergh[2], Ingmar Swart[2], and Cristiane Morais Smith[1]

[1] *Institute for Theoretical Physics, Utrecht University, Utrecht, the Netherlands*
[2] *Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, the Netherlands*

The dimensionality of a system is known to play an extremely important role in defining its electronic properties: in 3D electrons obey the Fermi-liquid paradigm, in 2D their charge becomes fractionalized in the presence of interactions and a strong perpendicular magnetic field, and in 1D one even observes a spin-charge separation. How electrons behave in fractional dimensions, however, has not been studied experimentally, simply because no geometric fractals exist in the quantum world. We have recently shown theoretically and experimentally that quantum fractals can be made by patterning the surface states of Cu(111) with CO adatoms. We realized Sierpinski gaskets up to 3 generations and found that the electronic wavefunction fractionalizes due to the geometric confinement. The experimental observations display an excellent agreement with muffin-tin and tight-binding theoretical predictions [1]. The same experimental and theoretical techniques were employed earlier to design a nano-Lieb lattice, which has no dual lattice and does not obey the triangular symmetry of the underlying copper substrate [2]. Our work opens up a myriad of new possibilities in engineering and characterizing novel quantum structures.

[1] S. N. Kempkes, M. R. Slot, S. E. Freeney, S. J. M. Zevenhuizen, D. Vanmaekelbergh, I. Swart, C. Morais Smith, arXiv:1803.04698.
[2] M. R. Slot, T. S. Gardenier, P. H. Jacobse, G. C. P. van Miert, S. N. Kempkes, S. J. M. Zevenhuizen, C. Morais Smith, D. Vanmaekelbergh, I. Swart, Nature Physics **13**, 672 (2017).

First-principles modeling of mixed-valence compounds from extended Hubbard-corrected functionals

Matteo Cococcioni and Nicola Marzari

Theory and Simulations of Materials (THEOS), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

An accurate characterization and understanding of transition-metal compounds, and especially of mixed-valence compounds, is central to many advanced applications in science and technology: from battery materials to photovoltaics, from multiferroics to deep-crust minerals. Unfortunately, first-principles approaches such as density-functional theory do not capture correctly the localization of valence electrons in low-dispersion states (e.g., d or f) and fail qualitatively and quantitatively in describing many properties of these systems. This work shows how extended Hubbard corrections to current functionals, including on-site (U) and inter-site (V) interactions, improve dramatically the description of the electronic, magnetic and structural properties, correctly describe localized states in the presence of significant inter-site hybridization, and capture exitations of charge-transfer character. Materials for Li-ion battery cathodes will be used as the main test case - showing how evaluating the effective interaction parameters consistently with the electronic and crystal structures greatly improves the prediction of thermodynamic quantities and of average voltages. Finally, I will show how to compute these interactions from density-functional perturbation theory, discussing how this approach ensures efficiency, accuracy, a streamlined protocol for automated calculations and, possibly, a suitable framework for the inclusion of frequency dependence.

Ultrafast modification of Hubbard U in a strongly correlated material: *ab initio* high-harmonic generation in NiO

N. Tancogne-Dejean[1], M. A. Sentef[1], and A. Rubio[1,2,3]

[1] *Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany*

[2] *Nano-Bio Spectroscopy Group and ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain*

[3] *Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010*

Engineering effective electronic parameters is a major focus in condensed matter physics. Their dynamical modulation opens the possibility of creating and controlling physical properties in systems driven out of equilibrium. In this work, we demonstrate that the Hubbard U, the on-site Coulomb repulsion in strongly correlated materials, can be modified on femtosecond time scales by a strong nonresonant laser excitation in the prototypical charge transfer insulator NiO. Using our recently developed time-dependent density functional theory plus self-consistent U (TDDFT+U) method, we demonstrate the importance of a dynamically modulated U in the description of the high-harmonic generation of NiO. Our study opens the door to novel ways of modifying effective interactions in strongly correlated materials via laser driving, which may lead to new control paradigms for field-induced phase transitions and perhaps laser-induced Mott insulation in charge-transfer materials.

Giant tuning of graphene's pseudospin polarization and valley splitting by a scanning tunneling microscope

Markus Morgenstern

II. Institute of Physics B and JARA-FIT, RWTH Aachen, 52074 Aachen, Germany

Graphene, the first two-dimensional material, provides two extra binary degrees of freedom, -sublattice and valley -, which are adequately described as a pseudospin. The sublattice pseudospin is chiral with respect to the Dirac-type momentum, such that it mimics the relativistic real spin completely. Here, I firstly show that application of large pseudomagnetic fields $B_p s$ (1000 T) can be used to polarize the sublattice pseudospin up to 40 precent. Therefore, the van-der Waals force of an STM tip is exploited, which locally lifts graphene from the SiO_2 substrate and, thus, induces huge strain gradients, i.e. $|B_p s|$. The resulting sublattice imbalance can be directly read from STM images and turns out to be in excellent agreement with analytic calculations based on molecular dynamics revealing the induced strain patterns [1]. Secondly, the valley degree of freedom is tuned using a quantum dot induced by the tip potential in combination with an external B field [2]. The laterally changing orientation of the graphene C atoms with respect to the B and N atoms on an angularly aligned BN substrate changes the valley splitting of the confined states continuously. This eventually leads to a tunable inversion of the valley splitting on nm length scales. Again, we provide excellent agreement with calculations, here, based on density functional theory combined with a tight binding model. [1] A. Georgi et al., Nano Lett., 17, 2240 (2017). [2] N. Freitag et al., Nano Lett., 16, 5798 (2016), Nat. Nanotechnol. 13, 392 (2018)

Validity of Weyl fermion picture for transition metals monopnictides TaAs, TaP, NbAs, and NbP from ab initio studies

Davide Grassano[1], Olivia Pulci[1], Adriano Mosca Conte[2], and Friedhelm Bechstedt[3]

[1] *Department of Physics, Universita' di Roma Tor Vergata, and INFN, Via della Ricerca Scientifica 1, I-00133, Rome, Italy*
[2] *Mediterranean Institute of Fundamental Physics (MIFP), Via Appia Nuova 31, I-00040, Marino, Rome, Italy*
[3] *IFTO, Friedrich-Schiller-Universität, Max-Wien Platz 1, D-07743, Jena, Germany. Correspondence and requests for materials should be addressed to O.P.*

In the past years topological insulators, with their peculiar protected surface states, have attracted a great deal of attention in the physics community[1]. Recently new classes for topologically relevant material have arisen. Among these are Weyl semimetals that show couples of nodes with linear band crossing close to the Fermi level with defined topological charge. One of the first proposed ways to realize them is by a multistacked structure of topological and trivial insulators with magnetic impurities[2]. These new materials can be seen as a tree-dimensional Dirac semimetals where either the time-reversal or inversion symmetries have been broken, leading to a lift of the degeneracy at the Dirac cone which splits into 2 Weyl nodes with defined chirality. These points are topologically protected and hence robust under perturbation. If we take a 2D slice of the material passing between two nodes of a pair, this will behave as a 2D topological insulator with chiral edge states crossing the Fermi level. By taking all the crossing points for all possible slices, a peculiar open Fermi surface for the surface states arise known as Fermi arc[3]. Transition metal monopnictides are a family of materials that crystallizes into a body centered tetragonal non symmorphic group which intrinsically lacks inversion symmetry. They have bee shown to be Weyl semimetals, both from ab initio and from experiments[4]. The aim of our work is to expand on the current ab initio results by performing detailed calculation of the low energy features in TaAs, TaP, NbAs and NbP. We compare our results with other ab initio and experimental data. We show how a simple Weyl fermion picture is not enough to describe the real properties of these systems where a more complex approach is required. We focus on the deviation of the optical properties from the expected linear trend and discuss the contribution to this effect from the tilt and anisotropy of the cones and from the presence of trivial points in the Brillouin Zone.

[1] MZ. Hasan et al,Reviews of Modern Physics 82.4 (2010):3045.
[2] AA. Burkov et al,Physical Review B 84.23 (2011):235126.
[3] X. Wan et al,Physical Review B 83.20 (2011):205101.
[4] SY. Xu et al,Science 349.6248 (2015):613-617.

The role of women in science: still a long way to go

Luisa Torsi

University of Bari, Italy

The statistics that concerns the percentage of women in apical positions in the academia in Europe still show a tremendous unbalance that see women strongly underrepresented. The problem is clear but the solutions are not trivial to find and to implement. The statistics published in “She Figures” (https://data.europa.eu/euodp/data/dataset/she-figures-2015-gender-in-research-and-innovation) will be shown and commented. The story of some prominent women scientists from the past will be also highlighted as examples of discriminations.

Why is physics still so gendered - and what can we do about it?

Tomas Brage

Department of Physics, Lund University, Sweden

Physics suffers from a two-dimensional segregation - both horizontal and vertical. This implies that women are not choosing Physics and that men are promoted faster and more efficient. These two effects are enhancing each other and leads to a domination of males especially in the leading positions. This talk will put forward some ideas on why this is still true, according to research in different fields. Solutions from recent studies and actions are proposed and discussed.

Applications of machine learning to materials science

Miguel A. L. Marques

Institute of Physics, Martin-Luther-Universität Halle-Wittenberg

In this talk I will summarize our recent attempts to apply machine learning techniques to the discovery and characterization of new materials. I will start by discussing the problem of stability of a given crystal phase. By generating large training and test sets, we benchmark the accuracy of several machines (regression trees, neural networks, etc.) to predict this quantity. We show that, by combining machine learning with traditional high-throughput techniques, one can obtain savings in computer time of the order of 75%. I then turn to the problem of the neural-network-based force fields, and show that training at the same time energies and forces yields much more reliable machines. This leads, unfortunately, for a much more complicated expression for the derivatives required for back-propagation. Finally, I will discuss the application of reinforcement learning techniques to the problem of quantum optimal control.

Predicting alloy properties, machine learning the gap between experiment and ab initio

M. J. van Setten[1,2,3], G. Petretto[1,2], G.-M. Rignanese[1,2], M. Marteleur[4], L. Choisez[4], and P. Jacques[4]

[1] *Nanoscopic Physics, Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, 1348 Louvain-la-Neuve, Belgium*
[2] *European Theoretical Spectroscopy Facility*
[3] *IMEC, Kapeldreef 75, Leuven*
[4] *Materials and process engineering, Institute of Mechanics, Materials and Civil Engineering, Université Catholique de Louvain, 1348 Louvain-la-Neuve, Belgium*

Engineering new materials with specific properties is often a tedious and expensive process. The preparation and characterization of a single sample may already take various days and can require sophisticated machinery. Finding an optimal candidate, moreover, requires a large search space including many samples. In principal, *ab initio calculations* can help in reducing the number of potential candidates. In practice two types of difficulties arise. To include complex, i.e. amorphous, heavily doped, or a multi component random alloy, materials in the search space makes these calculations very numerous and demanding. Moreover, the macroscopic property of interest may be difficult, if not impossible, to calculate in a direct way. In this work, we develop a method to solve these difficulties by using machine learning to connect complicated properties to simple calculations via a database of experimental results. The complicated properties are, in general, macroscopic in nature, like the type of mechanical deformation occurring under stress and need to be obtained for multi-component alloys. We couple these to descriptors derived as linear combinations of microscopic properties calculated for single stoichiometry two-component model systems. We apply this method to develop predictor models for the type of mechanical deformation occurring in titanium alloys. We build a database of 8 descriptors including 20 common doping elements. We investigate the space of microscopic descriptors and derive a subset by removing strongly correlating ones. With this subset we train various machine learning models and investigate which is most appropriate for this problem by comparing the predictions for newly obtained experimental results.

Structural prediction of free-standing 2-D materials

P. Borlido[1], M. Marques[2,3], and S. Botti[1,3]

[1] *Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany*
[2] *Institüt für Physik, Martin-LutherUniversität Halle-Wittenberg, D-06120 Halle (Saale), Germany*
[3] *European Theoretical Spectroscopy Facility*

Using a constrained global structural prediction method we performed an extensive investigation of the low density phases of two-dimensional carbon and silicon. As expected, we find that graphene is stable for a large range of biaxial strains, while more complex configurations becoming energetically more favorable at areas per atom above 3.12 Å^2. Two dimensional silicon presents a more complex phase diagram, which includes both haeckelite-like structures and dumbbell configurations. In particular, we find as the groundstate of two-dimensional silicon a novel structure formed by a honeycomb lattice with a few strategically positioned dumbbell atoms. This material is 218 meV/atom more stable than silicene and is a quasi-direct semiconductor with a band gap of around 1.11 eV and a very dispersive electron band. These properties should make it easier to synthesize than pristine silicene and interesting for a wealth of optoelectronic applications.

From one to three, exploring the rungs of Jacob's ladder in magnetic alloys

A. H. Romero[1] and M. J. Verstraete[2,3]

[1] *Department of Physics and Astronomy West Virginia University, Morgantown WV, USA*
[2] *nanomat/Q-MAT/CESAM, Universit é de Liège Belgium*
[3] *European Theoretical Spectroscopy Facility*

Magnetic systems represent an important challenge for electronic structure methods, in particular Density Functional Theory (DFT), which uses a single determinant wavefunction. To asses the predictions obtained by DFT in this type of materials, we benchmark different exchange correlation functionals with respect to each other, and with respect to available experimental data, on two families of binary iron alloys which are metallic and magnetic. We climb three rungs in Jacob's ladder of DFT (i) the local density approximation, (ii) the industry standard approximation due to Perdew, Burke and Ernzerhof, and the revised version for solids, PBEsol (iii) and finally a very accurate meta-GGA functional SCAN, which corresponds to the third rung. More than 350 structures in ferromagnetic and antiferromagnetic configurations were considered. We compare the Convex Hull, the calculated magnetic moment, crystal structure, formation energy and electronic gap if present. We conclude that none of the functionals work in all conditions: whereas PBE and PBEsol can give a fair description of the crystal structure and the energetics, SCAN strongly overestimates the formation energy - given values which are at least twice as large as PBE (and experiment). Magnetic moments are better predicted by PBE as well. Our results show that magnetic and strongly correlated materials are a tough litmus test for DFT, and that they represent the next frontier in the development of a truly universal exchange correlation functionals.

Electronic excitations in molecular solids from embedded many-body perturbation theory: fundamentals and applications

Gabriele D'Avino[1], Jing Li[1], Ivan Duchemin[2], David Beljonne[3], and Xavier Blase[1]

[1] *Institut Néel CNRS and Grenoble Alpes University, rue des Martyrs 25, F-38042 Grenoble, France*
[3] *INAC, SP2M/L Sim, CEA/UJF Cedex 09, F-38054 Grenoble, France*
[3] *University of Mons, place du Parc 20, BE-7000 Mons, Belgium*

The accurate description of charged (i.e. electron addition and removal) and optical excitations in complex, disordered and heterogeneous molecular solids, such as those of interest for organic electronics, represents a severe challenge for first-principles techniques. In this talk, we will introduce our novel hybrid quantum/classical (QM/MM) scheme merging many-body perturbation theory (GW formalism and Bethe-Salpeter equation) with accurate classical polarizable models of atomistic resolution.[1,2] Applications of this technique will be then discussed, starting from the photoelectron spectra of molecular solids, for which our embedded GW calculations, achieve quantitative accuracy in describing ionization energies and electron affinities of different molecular crystals, shedding light on the interplay between dielectric screening, electrostatic crystal field effects and band dispersion.[2] We will then consider chemical impurities, such as the strong electron-acceptor F4TCNQ, in the pentacene crystal, which represents a paradigmatic case of p-doping in organic semiconductors.[3] Our calculations show that dopants can ionize at room temperature in spite of impurity acceptor levels lying very deep in the gap. The excitonic interaction is crucial for the dopant ionization, yet this process leads to a charge carrier that is strongly Coulombically pinned to the impurity. Our findings reconcile apparent contradictions in the experimental literature, shedding light on the first steps of the doping mechanism.[3]

[1] J. Li, G. D'Avino, I. Duchemin, D. Beljonne, X. Blase, J. Phys. Chem. Lett. 7, 2814 (2016)
[2] J. Li, G. D'Avino, I. Duchemin, D. Beljonne, X. Blase, Phys. Rev. B 97, 035108 (2018)
[3] J. Li, G. D'Avino, A. Pershin, D. Jacquemin, I. Duchemin, D. Beljonne, X. Blase, Physical Review Materials, 1, 025602 (2017)

Computational spectrosocpy at finite temperature

Giulia Galli

University of Chicago and Argonne National Laboratory

We will discuss several electronic properties of interfaces and disordered systems carried out by coupling first principles molecular dynamics (in particular the Qbox code) and excited states calculations (in particular the WEST code).

Free surfaces recast superconductivity in fewmonolayer MgB2: Combined first-principles and ARPES demonstration

J. Bekaert[1], L. Bignardi[2,3], A. Aperis[4], P. van Abswoude[2], C. Mattevi[5,6], S. Gorovikov[7,8],
L. Petaccia[7], A. Goldoni[7], B. Partoens[1], P. M. Oppeneer[4], F. M. Peeters[1], M. V. Milosević[1],
P. Rudolf[2], and C. Cep

[1] *Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium.*
[2] *Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747AG Groningen, The Netherlands.*
[3] *Present address: Elettra Sincrotrone Trieste, Strada Statale 14 km.163.5, I-34149 Trieste, Italy.*
[4] *Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden.*
[5] *IOM-CNR, Laboratorio TASC, Strada Statale 14 km.163.5, I-34149 Trieste, Italy.*
[6] *Present address: Department of Materials, Imperial College London, Exhibition road, SW7 2AZ, London, United Kingdom.*
[7] *Elettra Sincrotrone Trieste, Strada Statale 14 km.163.5, I-34149 Trieste, Italy.*
[8] *Present address: Canadian Light Source Inc., 44 Innovation Blvd, Saskatoon, SK S7N 2V3, Canada.*

Two-dimensional materials are known to harbour properties very different from those of their bulk counterparts. Recent years have seen the rise of atomically thin superconductors, with a caveat that superconductivity is strongly depleted unless enhanced by specific substrates, intercalants or adatoms. Surprisingly, the role in superconductivity of electronic states originating from simple free surfaces of two-dimensional materials has remained elusive to date. Here, based on first-principles calculations and angle-resolved photoemission spectroscopy (ARPES), we show that surface states in few-monolayer MgB2 make a major contribution to the superconducting gap spectrum and density of states, clearly distinct from the widely known, bulk-like σ- and π-gaps. As a proof of principle, we predict and measure the gap opening on the magnesium-based surface band up to a critical temperature as high as $\tilde{3}0$ K for merely six monolayers thick MgB2. These findings establish free surfaces as an unavoidable ingredient in understanding and further tailoring of superconductivity in atomically thin materials [1].

[1] J.Bekaert et al., Scie.Rep. 7, 14458 (2017)

DFT & electron holography

Z. Zanolli[1,2]

[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus Bellaterra, 08193 Barcelona, Spain*

[2] *European Theoretical Spectroscopy Facility (ETSF)*

The quantitative analysis of electron-optical phase images recorded using off-axis electron holography often relies on the use of computer simulations of electron propagation through a sample. However, simulations that make use of the independent atom approximation are known to overestimate experimental phase shifts by approximately 10%, as they neglect bonding effects. Here, we compare experimental and simulated phase images for few-layer WSe_2. We show [1] that a combination of pseudopotentials and all-electron density functional theory calculations can be used to obtain accurate mean electron phases, as well as improved atomic-resolution spatial distribution of the electron phase. The comparison demonstrates a perfect contrast match between experimental and simulated atomic-resolution phase images for a sample of precisely known thickness. The low computational cost of this approach makes it suitable for the analysis of large electronic systems, including defects, substitutional atoms and material interfaces. [1] S. Borghardt, F. Winkler, Z. Zanolli, M. J. Verstraete, J. Barthel, A. H. Tavabi, R. E. Dunin-Borkowski, and B. E. Kardynal, Phys. Rev. Lett. 118, 086101 (2017)

New developments for resonant Raman scattering and phonon-assisted indirect absorption/emission

Ludger Wirtz, Fulvio Paleari, Sven Reichardt, Henrique Miranda, and Alejandro Molina-Sánchez

Physics and Materials Science Research Unit, University of Luxembourg

We present our recent progress in the development of diagrammatic perturbation theory for resonant Raman spectroscopy and for phonon-assisted indirect absorption. The goal is a consistent theory that takes into account excitonic effects and dynamic effects of electron-phonon coupling. We compare numerical implementations based on a finite difference approach with implementations of perturbation theory. Our approach enables us to understand the resonant Raman spectra of multi-layer transition-metal dichalcogenides and the complex luminescence spectra of bulk boron nitride.

Cumulant expansion of the electronic polarizability: beyond the static Bethe-Salpeter equation

Pierluigi Cudazzo[1] and Lucia Reining[2]

[1] *University of Luxembourg*
[2] *LSI, École Polytechnique, Palaiseau (France)*

One of the big challenges of theoretical condensed matter physics is the description, understanding, and prediction of the effects of the electronic correlations induced by the mutual interaction between particles on materials properties. In both electronic and optical spectra the Coulomb interaction causes a renormalization of the energies and change of spectral weight. Most importantly, it induces a finite lifetime on the quasi-particle (QP) excitations and can lead to new structures, often called satellites. The latter are pure many body effects and can be linked to the coupling of excitations, also termed dynamical effects. Standard methods developed in the framework of many body perturbation theory namely GW and the Bethe-Salpeter equation (BSE) are often not able to capture this complex physics. Instead, approaches based on a picture of electron-boson coupling such as the cumulant expansion are promising for the description of plasmon satellites. Motivated by the recent success of the cumulant expansion of the one particle Green's function in the description of photoemission spectra[1, 2,3], we generalized the cumulant approach to the evaluation of the electronic polarizability. In this way we provide a new full ab-nitio tool to include dynamical effects beyond the standard BSE in the description of neutral excitations as measured in optical absorption, electron energy loss and inelastic X-rays scattering spectroscopies.

[1] M. Guzzo, et al., Phys. Rev. Lett. 107, 166401 (2011).
[2] J. Lischner, D. Vigil-Fowler, and S. G. Louie, Phys. Rev. Lett. 110, 146801 (2013).
[3] J.S. Zhou, et al., J. Chem. Phys. 143, 184109 (2015).

Invisible excitations in hexagonal Boron Nitride

C. Attaccalite[1,2], L. Sponza[3], M. Grüning[4], H. Amara[3], and F. Ducastelle[3]

[1] *CNRS/Aix-Marseille Université CINAM, Campus de Luminy, Maseille (France)*
[2] *University of Rome Tor Vergata, Rome, Italy*
[3] *LEM, UMR 104 CNRS-ONERA, Universite Paris Saclay F-92322 Chatillon, France*
[4] *School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK*

In this talk I will describe excitations in hexagonal boron nitride that are not visible in the optical response. In particular I will focus on electron-loss spectroscopy[1], and show that this technique can reveal the indirect nature of h-BN. Then I will discuss two-photon absorption as possible tool to probe dark states below the bright exciton of the h-BN[2]. These states have a strong implication for luminescence properties of this material.

[1] Exciton interference in hexagonal boron nitride L. Sponza, H. Amara, F. Ducastelle, A. Loiseau, C. Attaccalite, Physical Review B 97 (7), 075121 (2018)
[2] Two-photon absorption in two-dimensional materials: The case of hexagonal boron nitride C. Attaccalite, M. Grüning, H. Amara, S. Latil, F. Ducastelle, arXiv preprint arXiv:1803.10959

Quantum Chemical Simulations of Stimuli–Responsive Nanomaterials for Biomedical Applications

C. Di Valentin, D. Selli, H. Liu, and M. Kaviani

Università di Milano Bicocca, Dipartimento di Scienza dei Materiali, via Cozzi 55, Milano, Centro di Nanomedicina, via Cadore 48, Monza, Italy

In this talk, I will present an overview on our computational activity devoted to nanohybrid systems based on transition metal oxide nanoparticles (i.e. TiO_2 and Fe_3O_4) and graphene oxide flakes for biomedical applications. Atomic models of realistic size (2—4 nm, i.e. 800—4000 atoms) are used to simulate, at a quantum mechanical level of theory, the structural, electronic and magnetic properties of the nanosystems, their interaction with light and with the aqueous environment. Further surface functionalization with stabilizing polymers or functionalizing species for drug delivery is then discussed.

End-group effects in tuning the semiconductor-to-metal transition of carbon atom wires: insights from first-principles calculations

Alberto Milani[1], Matteo Tommasini[2], Chiara Castiglioni[2], Valeria Russo[1], Andrea Li Bassi[1], and Carlo S. Casari[1]

[1] *Dip. Energia, Politecnico di Milano, Via Ponzio 34/3 - 20133, Milano, Italy*
[2] *Dip. Chimica, Materiali, Ing. Chimica, Politecnico di Milano, P.zza Leonardo da Vinci 32 - 20133, Milano, Italy*

Carbon-atom wires (CAWs) are linear, finite-length molecules, whose ideal limit is the so-called “carbyne”, a 1-D carbon allotrope displaying outstanding theoretical properties [1,2]. Similar to other polyconjugated systems, CAWs display structural, electronic and optical properties which depend on their length and type of end-groups. Therefore, such properties can be tuned over the insulating-semiconducting-metallic behavior. For this reason, CAWs offer an appealing opportunity for developing novel functional nanostructures. Two different reference classes of CAWs have been identified: polyynes (bond-length-alternated chains with insulating/semiconducting character), and cumulenes (more equalized systems with nearly metallic behavior). On these grounds, a fundamental and open issue regards how and to what extent the properties of CAWs can be effectively modulated by controlling π-electron conjugation. In this contribution, we explore CAWs terminated by different kinds of end-groups (sp^2-carbon groups and donor-acceptor moieties). In particular, Density Functional Theory is employed to predict the electronic gap, the degree of bond length alternation (BLA) and the Raman response as a function of the structure of the chain and/or the occurrence of charge transfer effects, to reveal the occurrence of a polyyne-to-cumulene transition. The computed spectroscopic response is compared with available experimental Raman and SERS spectra of most of the systems here investigated. First, we investigate the effect of different sp^2 end-groups, starting from CAWs terminated by two biphenyl groups and then generalizing the discussion to highlight the role of aromatic end-groups of increasing size (i.e., phenyl, biphenyl, naphthyl, and coronene, also with oxygen substituents). The increase of sp^2 conjugation alone is found to be not enough to endow the full tunability of properties. Instead, a wide range tunability can be obtained by controlling charge transfer effects or by proper chemical design (i.e., oxygen substitution or adoption of cumulene-inducing terminations) [3]. Second, previously synthetized donor/acceptor CAWs are investigated and reveal how charge transfer is properly modulated by both the sp-carbon chain length, and the peculiar functional groups added to the chains, which imparts a subtle influence on the structural/electronic/spectroscopic properties. These results provide a guideline for the design of novel nanostructures based on CAWs, including both sp-sp^2 hybrid systems where graphene-like and polyyne-like domains are closely interconnected, or donor/acceptor systems including heteroatoms. The capability to tune the final electronic or optical response of the material makes all these systems appealing for a future carbon-based science and technology.

[1] C.S. Casari et al. Nanoscale **8**, 4414 (2016)
[2] C.S. Casari, A. Milani MRS Comm. (2018) doi:10.1557/mrc.2018.48
[3] A. Milani et al. J. Phys. Chem. C **121**, 10562 (2017).

Impact of alkali metal-doping on the electronic and optical properties of organic molecules adsorbed on metal surface

Anu Baby[1], Marco Gruenewald[3], Christian Zwick[3], Tino Kirchhuebel[3], Felix Otto[3], Roman Forker[3], Benjamin Stadtmüller[4], Christian Kumpf[5], Gian-Paolo Brivio[1], Guido Fratesi[6], Egbert Zojer[2], and Torsten Fritz[3]

[1] *Department of Materials Science, University of Milano-Bicocca, Via R. Cozzi 55, 20125 Milano, Italy*
[2] *Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria*
[3] *Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany*
[4] *University of Kaiserslautern, Erwin-Schrödinger-Strasse 1, 67663 Kaiserslautern, Germany*
[5] *Forschungszentrum Jülich, 52425 Jülich, Germany*
[6] *Dipartimento di Fisica, Universitá degli Studi di Milano, Via Celoria 16, 20133, Milano, Italy*

We study the impact of K doping of a PTCDA (sub)monolayer domain on Ag(111) to gain profound insights onto the doping-induced changes of the optical and electronic properties of the interface [1,2]. A particular advantage of the KxPTCDA/Ag(111) system is that it is known to form distinct stoichiometric phases, which allows associating the observed spectra with well-defined adsorbate structures. Unfortunately, the interpretation of the measured differential reflectance spectra is highly ambiguous, which prompted us to perform state-of-the-art density-functional theory based calculations using VASP and Quantum Espresso. The optical spectra was calculated at the IPRPA (Independent particle random phase approximation) level using Yambo software. These provide an atomistic understanding of the interfacial charge rearrangements and in conjunction with photoelectron spectra and X-ray standing wave data allow a comprehensive explanation of the interface properties. Full structural characterization is obtained by low-energy electron diffraction and scanning- tunneling microscopy experiments [2]. The presence of the K atoms is found to increase the electron density in the organic layer and in the Ag substrate; at the same time it reduces the coupling between the adsorbate and the substrate. The latter, on the one hand, is evidenced by the decreasing dispersion and hybridization of the PTCDA-derived bands in potassium-rich phases and, on the other hand, can be concluded from an increasing adsorption distance and reduced optical spectra peak widths upon K intercalation found in both theory and experiments. Results for the K doped tetraphenyldibenzoperiflanthene (DBP) on Ag(111) will be presented as well. Undoped DBP is a donor whereas undoped PTCDA is an acceptor when adsorbed on Ag(111). Hence these two systems provide full understanding of well-defined metal-organic interface in the presence of alkali atoms both when the organic molecule has donating and/or accepting character, which will be useful as a benchmark for future studies.

[1] Anu Baby, et al., ACS Nano, 11, 10495–10508 (2017).
[2] Zwick, et al. ACS Nano, 10, 2365–2374 (2016).

Why Silicon is not Carbon?

M. Pizzochero[1], M. Bonfanti[2], and R. Martinazzo[3,4]

[1] *Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*
[2] *Institute of Physical and Theoretical Chemistry, Goethe Universität Frankfurt, Max-von-Laue-Str. 7, 60438 Frankfurt, Germany*
[3] *Department of Chemistry, Università degli Studi di Milano, via Golgi 19, 20133 Milan, Italy*
[4] *Institute of Molecular Science and Technologies (ISTM), Consiglio Nazionale delle Ricerche (CNR), Milan, Italy*

Despite their formal similarity, the structure, the stability and the chemical properties of unsaturated molecules containing higher main group elements are strikingly different from their first row counterparts. This is particularly evident when comparing Si and C, in any of their molecular or extended form, since the extraordinary chemical flexibility of carbon which is at the basis of the known living matter is not shared by its congeners. The size of the atoms, the effective extensions of the s and p shells and their energetic separation have been invoked to explain some of the unique chemical properties of first row elements but none of these features can explain the simple differences that arise in the structure of π bonded atoms. Here, focusing on the Si *vs.* C comparison (and including Ge to some extent), we argue that electron correlation plays a major role in higher main group elements, despite the e-e repulsion is smaller on an absolute scale for the heavier atoms. We show that a structural instability arises for π-bonded Si and Ge atoms because they are closer than C to a Heitler-London limit where the atoms acquire radical character. Hence, upon artificially weakening the effective e-e repulsion in the p shell one may completely remove such instability and turn Si and Ge into closer relatives of C than they are used to be.

GeV$_n$ defects in silicon: a viable route toward high temperature single electron transport

S. Achilli[1], N.Manini[1], G. Onida[1], T. Shinada[2], T. Tanii[3], and E. Prati[4]

[1] *Universitá degli Studi di Milano, Dipartimento di Fisica, Via Celoria 16, 20133 Milano.*
[2] *Center for Innovative Integrated Electronic Systems, Tohoku University, 468-1 Aramaki Aza Aoba, Aoba-ku, 980-8572 Sendai, Japan.*
[3] *Faculty of Science and Engineering, Waseda University, 3-4-1 Ohkubo, Shinjuku, 169-8555 Tokyo, Japan.*
[4] *Istituto di Fotonica e Nanotecnologie, Consiglio Nazionale delle Ricerche, Piazza Leonardo da Vinci 32, 20133 Milano, Italy.*

Single-atom transistors are the ultimate scaling solution for applications in quantum information. Devices based on conventional dopant atoms (As, P) in silicon can operate only at cryogenic temperature due to shallow weakly localized impurity levels. Ge dopants are promising candidates for operating single electrons at room temperature, forming stable defect complexes with single or multiple vacancies, characterized by very deep levels in the energy gap. By means of ab initio DFT calculation with screened-exchange hybrid functional, that solves the “gap and delocalization problem” of standard DFT, we characterize structural and electronic properties of different Ge-V$_n$ defects. We compute the adiabatic and thermodynamic charge transition levels corresponding to the excitation energies for the addition of electrons to the defect. We show that the energy position of these excited states in the gap and their localization on the defects may shed light on the physics behind the features observed in the experimental I-V curves and on the electron transport mechanisms in the system.

Nonadiabatic Dynamics in Single-Electron Tunneling Devices with Time-Dependent Density-Functional Theory

Niklas Dittmann[1,2,3], Janine Splettstoesser[1], and Nicole Helbig[2,3]

[1] *Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, SE-41298 Göteborg, Sweden*

[2] *Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany* [3] *Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*

We simulate the dynamics of a single-electron source, modelled as a quantum dot with on-site Coulomb interaction and tunnel coupling to an adjacent lead in time-dependent density-functional theory. Based on this system, we develop a time-nonlocal exchange-correlation potential by exploiting analogies with quantum-transport theory. The time nonlocality manifests itself in a dynamical potential step. We explicitly link the time evolution of the dynamical step to physical relaxation time scales of the electron dynamics. Within linear response the new functional shows a linear dependence of the exchange-correlation kernel on the frequency. Finally, we discuss prospects for simulations of larger mesoscopic systems.

An ab-initio approach to describe coherent and non-coherent exciton dynamics

Davide Sangalli[1,3], Enrico Perfetto[1,3], Gianluca Stefanucci[2,3], and Andrea Marini[1,3]

[1] *CNR-ISM, Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy*
[2] *Dipartimento di Fisica, Università di Roma Tor Vergata, and INFN, Sezione di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy*
[3] *European Theoretical Spectroscopy Facility (ETSF)*

The use of ultra–short laser pulses to pump and probe materials activates a wealth of processes which involve the coherent and non coherent dynamics of interacting electrons out of equilibrium. Non equilibrium (NEQ) many body perturbation theory (MBPT) offers an equation of motion for the density–matrix of the system which well describes both coherent and non coherent processes. In the non correlated case there is a clear relation between these two regimes and the matrix elements of the density–matrix. The same is not true for the correlated case, where the potential binding of electrons and holes in excitonic states need to be considered. In the present work we discuss how NEQ-MBPT can be used to describe the dynamics of both coherent and non-coherent excitons in the low density regime. The approach presented is well suited for an ab initio implementation. [1,2]

[1] D. Sangalli et al., arXiv:1803.01200 (2018), just accepted on EPJB
[2] E. Perfetto et al., Physical Review B **94**, 245303 (2016)

Poster contributions

Efficient modelling of band alignments in a semiconductor/alloy interface

J. Abreu[1], G. Greene-Diniz[1], and M. Gruening[1]

[1] *Queen's University Belfast*

The semiconductor/alloy interface is the key to control the performance of new electronic and optoelectronic devices. The electronic property I will focus is the bands offset, important for macroscopic transport mechanisms and some important parameters that affect this property can be the stoichiometry composition, elastic deformations, and atomic diffusion in the interface[1,2]. When a hetero-junction forms, atoms from on material can diffuse to another and modify the bands offset[3]. Besides, some materials have interesting enhancement when they are strained, as is the case of Germanium which can become direct band gap semiconductor[4]. So a controlled tensile strain would be useful to improve the performance of the device, which can be done by changing the concentration elements of the alloy and this can also alter the bands offset. Another effect on the bands offset are the bonds in the interface, changing the stoichiometry composition may change an interface of straddling type (I) to an interface of staggered type (II). Here we study the case of the interface of ϵ—Ge/In$_x$Ga-$_{1-x}$As which is relevant for tunnel field effect transistor [5]. A study of the bands offset is done by calculating the average electrostatic potential in a supercell with the interface together with the calculation of the band gaps of each material in bulk. The alloy composition is generated by special quasirandom structure that mimics a random alloy. [6]

[1] M. Peressi, N. Binggeli, A. Baldereschi, J. Phys. D: Appl. Phys. **31** (1998)
[2] M. Giantomassi et al., Phys. Status Solidi B **248** (2011)
[3] P. Rodigues-Hernandez, A. Mujica, A. Munoz, Physica B: Phys. Cond. Mat. **185** (1993)
[4] J. J. Sanchez-Perez et al, PNAS **108**, 47 (2011)
[5] A. M. Ionescu, H. Riel, Nature **479** (2011)
[6] S.H. Wei, L. G. Ferreira, J. E. Bernard, A. Zunger, Phys. Rev. B **42**, 15 (1990)

Strain Induced NDR and Rectification Behavior on The γ- Graphyne Nanotubes

Aidin Ahmadi , Homayoun Jafari, and Mahdi Faghihnasiri

Young Researchers and Elite Club, South Tehran Branch, Islamic Azad University, Tehran, Iran. Department of Physics, Iran University of Science and Technology, Tehran, Iran. Computational Materials Science Laboratory, Nano Research and Training Center, NRTC,Iran.

The current-voltage characteristics of three different diameters armchair and zigzag γ-graphyne nanotubes under uniaxial strain are investigated by using first-principles quantum transport calculations through density functional theory and non-equilibrium Green's function method. It is shown that for a given value of bias voltage, the resulting current depends strongly on the applied load so that tensile and compressive strain can generate Negative Differential Resistance (NDR) mostly into the armchair nanotubes. Our study reveals that the rectification behavior of the systems is mainly due to the asymmetric electron transmission function distribution in the conduction and valence bands.

The connector theory: new approximations for the exchange-correlation potential

A. Aouina[1,2], M. Gatti[1,2], and L. Reining[1,2]

[1] *Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, F-91128 Palaiseau, France*

[2] *European Theoretical Spectroscopy Facility (ETSF)*

The "connector theory" is a novel strategy that we have recently introduced [1] to design systematic approximations. It is a general prescription to import, in principle exactly, a quantity of interest froma model into a real system. An enormous advantage is that model results can be obtained once forever and tabulated. Here we focus on the exchange-correlation (xc) potential of density-functional theory (DFT) [2], including the time-dependent (TD) case, and we use the homogeneous electron gas (HEG) as the model system. We illustrate why the connector theory constitutes a better scheme for approximations than an approach that would directly approximate the xc potential. By making use of advanced calculations for the TDDFT xc kernel of the HEG [3], we derive xc potentials that have a non-local density dependence and are non-adiabatic. We consider simple examples and we compare the results of our approach with those of the local-density approximation (LDA). We highlight the differences and we show why our theory is a promising approach of approximation.

[1] M. Vanzini, A. Aouina, M. Panholzer, M. Gatti, and L. Reining, in preparation.
[2] W. Kohn, Rev. Mod. Phys. 71, 1253 (1999).
[3] M. Panholzer, M. Gatti, and L. Reining, Phys. Rev. Lett. 120, 166402 (2018)

Chemical reactions by STM: a new way to synthetize tetra-aza-pentacene(TAP)

C. Attaccalite, T. Leoni, T. Lelaidier, A. Thomas, A. Ranguis, O. Siri and C. Becker

CNRS/Aix-Marseille Université CINAM, Campus de Luminy, Maseille (France)

In this work we take advantage of the STM (scanning tunneling microscopy) to overcome the limit of conventional organic chemistry in the synthesis of tetraazapentacene (TAP). All previous studies devoted to the synthesis of TAP with no substituent in solution failed. This synthesis of TAP remains a major challenge in chemistry because of the effective application in organic electronic predicted for this molecule. Starting from self-assembled layer of DHTAP (dihydroaza-pentacene) on Au(111), we perform voltage pulse on individual molecule in order to populate the LUMO of the addressed molecule. This molecule-induced resonant state can relax via the excitation of a molecular vibration that leads to the dissociation of N-H bond. We use high resolution STM image to analyze the result of our voltage pulse combined with DFT calculation of the molecular orbitals. We demonstrate that DHTAP can undergo single or double dehydrogenation resulting in a TAP molecule. We show that this single molecule on surface synthesis can be extended to a larger area by using STM in field emission mode. These preliminary works suggest that technological applications of TAP layers might be possible after the dehydrogenation of DHTAP.

Ab-initio Many Body Perturbation Theory approaches for the calculation of electronic properties of cyclometalled Ir(III) complexes

Marco Cazzaniga, Marta Penconi, Fausto Cargnoni, Alberto Bossi, and Davide Ceresoli

Istituto di Scienze e Tecnologie Molecolari - CNR, via Golgi 19, I-20133 Milan (Italy)

The wide commercial interest in Organic Light Emitting Diodes motivate the development of new phosphorescent emitters, usually belonging to the class of Ir(III) cyclometalled compounds. Indeed the presence of the metallic center with a careful design of the surrounding ligands allow to obtain phosphorescent emission at the desired wavelength. In order to provide an interpretation of the large amount of available experimental data, usually their discussion is supported by theoretical calculation generally based on TDDFT with the use of hybrid functionals like the B3LYP. Anyway the good agreement with measured spectra, which explains the success of this approach, can be seen somehow fortuitous. On the contrary, due to the dimensions of these compounds the application more complex quantum chemistry approaches can become challenging. An alternative solution comes from the Many Body Perturbation Theory and from the recently available implementations of the GW approximation and of the Bethe-Salpeter equation in gaussian basis set. In the present work we will apply these approaches for the calculation of the quasiparticle energies and optical absorption of 6 standard Cyclometalled Ir(III) complexes whose emission frequencies are scattered around the visible range. Additionally we choose Ir(ppy)$_3$ as a template to investigate in detail the effect of the DFT starting point and the effect of the eigenvalue self-consistency in the GW calculations.

Ab-initio molecular dynamics simulations of excitation-induced OLED degradation

Marco Cazzaniga, Marta Penconi, Alberto Bossi, Davide Ceresoli, and Fausto Cargnoni

Istituto di Scienze e Tecnologie Molecolari - CNR, via Golgi 19, I-20133 Milan (Italy)

The use of phosphorescent organic molecules in OLEDs offers the potential of using both the singlet and triplet excitons in realizing 100% internal quantum efficiency of electro-luminescence. However, the injected charge carriers (electrons and holes) may become trapped, thus yielding to the accumulation of non-radiative recombination centers and luminescence quenchers at morphological and chemical defects, yielding, in the worst cases, to chemical degradation of the adopted materials. In order to shed light on the dissociation pathways, we performed Car-Parrinello molecular dynamics with constrained orbital occupations to simulate the presence of an excitation (electron, or hole polaron and an electron-hole exciton), as if it were electrically injected into the device. We applied that approach to few molecules used in OLEDs both as host material (CBP aNPD and mCP) and as phosphorescent emitter (FIrpic). In particular, for the last one we were able to observe the dissociation of a ligand in presence of an exciton. Additionally, following the CP results, we determined the dissociation energies of few relevant bonds with more advanced methods.

Electric and magnetic response properties of solids from the current density

R. Ferradás[1], P. Romaniello[2], and J. A. Berger[1]

[1] *Laboratoire de Chimie et Physique Quantiques, IRSAMC, Université de Toulouse, CNRS, UPS, France*
[2] *Laboratoire de Physique Théorique, IRSAMC, Université de Toulouse, CNRS, UPS, France*

The evaluation of the macroscopic polarization and magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities [1,2]. In this work we show the advantage of calculating electric and magnetic response properties of solids using the current density as basic variable. An efficient approach to calculate the current density is time-dependent current-density-functional theory (TDCDFT). In TDCDFT the electron current-density enters, replacing the electron density of ordinary TDDFT as the fundamental dynamical variable, with a vector potential instead of a scalar potential as its conjugate variable. We will show results for optical properties [3] of solids using a recently developed functional [4]. We will finally discuss how magneto-optical properties can be addressed within this framework.

[1] F. Kootstra, P.L. de Boeij and J.G. Snijders, J. Chem. Phys. **112**, 6517 (2000)
[2] P. Romaniello and P.L. de Boeij, Phys. Rev. B **71**, 155108 (2005)
[3] R. Ferradás, J.A. Berger and P. Romaniello, Eur. Phys. Jour. B, in press
[4] J.A. Berger, Phys. Rev. Lett. **115**, 137402 (2015)

New method for computing band gaps from grand canonical quantum Monte Carlo calculations applied to solid hydrogen.

Vitaly V. Gorelov[1], Markus Holzmann[2,3], D. M. Ceperley[4], D. Domin[1], and Carlo Pierleoni[1,5]

[1] *Maison de la Simulation, CEA, CNRS, Univ. Paris-Sud, UVSQ, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*
[2] *Univ. Grenoble Alpes, CNRS, LPMMC, 3800 Grenoble, France*
[3] *Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex 9, France*
[4] *Department of Physics, University of Illinois Urbana-Champaign, Illinois, USA*
[5] *Department of Physical and Chemical Sciences, University of L'Aquila, Italy*

We propose a purely variational method for computing band gaps within quantum Monte Carlo (QMC) simulation. Based on grand canonical reptation quantum Monte Carlo (GC-RQMC) with twisted boundary conditions, we analyze energies of systems of N_p protons varying the number of electrons, N_e, from $N_p - \Delta N$ to $N_p + \Delta N$. Total neutral magnetization is assured by adding/subtracting always even number of electrons whereas odd numbers probe spin excitations. Grand canonical analysis can be done as a post processing converting the dependency on the number of electrons N_e in favour of the chemical potential μ. Different twists are used to correct all single particle size effects, two-particle size effects are corrected by analyzing the structure factor $S(k,\mu)$ [1]. We apply this new technique to compute the band gap of solid molecular hydrogen beyond 250 GPa. We investigate two candidate structures of phase III: C2/c and Cmca12 [2]. For these crystalline structures at zero temperature the band gap closes above 400 GPa, for the Cmca12 at slightly lower pressure than for the C2/c. We also show that the size effects for the value of a band gap are not that strong as it was shown before. From the variation of the momentum distribution $n(k,\mu)$ with respect to the chemical potential, we argue that the band gap is indirect. These results are in reasonable agreement with predictions based on QMC corrected Density Functional Theory (DFT) [3]. Our purely QMC based method allows us to gain more understanding and better insight from a many-body prospective without relying on a specific DFT functional. Furthermore, our scheme can be straightforwardly applied to more general situations including thermal and zero point motion of protons beyond the harmonic approximation.

[1] M.Holzmann, R.C.Clay, M.A.Morales, N.M.Tubman, D.M.Ceperley and C.Pierleoni, Phys. Rev. B **94(3)** , 035126 (2016).
[2] G. Rillo, M. A. Morales, D. M. Ceperley, and C. Pierleoni, J. Chem. Phys. **148** , 102314 (2018).
[3] S. Azadi, N. D. Drummond and W. M. C. Foulkes, Phys. Rev. B **95**, 035142 (2017).

First principles calculations of band offsets at heterovalent ε-Ge/In$_x$Al$_{1-x}$As interfaces

G. Greene-Diniz and M. Grüning

Atomistic Simulation Centre, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom

Tensile strained Ge (ε-Ge) grown on III-V substrates is currently the focus of substantial research efforts due to the range of potential technological applications, from high performance, low power tunnel FETs, to on-chip optical interconnects based on III-V/ε-Ge/III-V quantum well light emitters. In this work, we investigate the sensitivity of quasiparticle band offsets to interface structure for the ε-Ge/(001)In$_x$Al$_{1-x}$As interface. Utilizing first principles methodologies for atomistic simulations, namely density functional theory (DFT) combined with many body perturbation theory within the GW approximation, valence and conduction band alignments are calculated for a range of interface configurations. Considering the combined effects of cation stoichiometry of the substrate, interface stoichiometry, diffusion of mixed layers across the interface, and the strain induced movement of quasiparticle valleys in Ge, band alignments recently measured from core level XPS spectra for epitaxial thin films of ε-Ge on (001)In$_{0.25}$Al$_{0.75}$As substrates are explained in terms of the of diffusion of substrate species into the Ge film.

Nonlinear optics in dielectrics from first-principles

Myrta Grüning[1,2] and Claudio Attaccalite[2,3]

[1] *Queen's University Belfast*
[2] *European Theoretical Spectroscopy Facility*
[3] *CNRS/Aix Marseille Université and Univerità Roma Tor-Vergata*

We review a first-principles real-time approach to calculate nonlinear optical properties in dielectrics [1] and showcase results obtained with this approach for the second- and third-harmonic generation and two-photon absorption in bulk crystals, 2D materials and nanostructures [2,3,4,5] at different level of theory [6,7].

[1] C. Attaccalite and M. Grüning Phys. Rev. B 88, 235113 (2013)
[2] Claudio Attaccalite, Myrta Grüning, Hakim Amara, Sylvain Latil, François Ducastelle arXiv:1803.10959
[3] C. Attaccalite, E. Cannuccia, and M. Grüning Phys. Rev. B 95, 125403
[4] C. Attaccalite, A. Nguer, E. Cannuccia, and M. Grüning Phys. Chem. Chem. Phys. 17 9533 (2015)
[5] M. Grüning and C. Attaccalite Phys. Rev. B 89, 081102(R); Phys. Rev. B 90, 199901 (2014)
[6] M. Grüning, D. Sangalli, and C. Attaccalite Phys. Rev. B 94, 035149; M. Grüning and C. Attaccalite Phys. Chem. Chem. Phys., 2016,18, 21179-21189
[7] C. Attaccalite, M. Grüning, and A. Marini Phys. Rev. B 84, 245110

Analysis and Optimization of nanoscale III-Nitride heterostructure field effect transistors with a gate field-plated

M. Kaddeche[1], A. Telia[2], and A. Soltani[3]

[1] *Département de Technologie, Faculté des Sciences et de la Technologie Université de Djilali Bounaâma-Khemis miliana, Ain Defla -Algeria(*email: kaddeche@gmail.com)*

[2] *Laboratoire de Microsystème et Instrumentation (LMI), Département d'électronique, Université Mentouri de Constantine, 25000 Constantine, Alegria*

[3] *IEMN-CNRS 8520, Université des Sciences et Technologie de Lille, Cité Scientifique avenue Poincaré 59655 Villeneuve d'ascq- France*

The excellent microwave power performance demonstrated in AlGaN/GaN HEMTs (high-electron mobility transistors) results from the combination of high current density with high voltage operation [1], which benefits from the high sheet charge density in these hetero-structures (1013 cm-2), the high carrier mobility (1500 cm2/Vs) and saturation velocity (1.5 × 107 cm/s) in the channel and the high breakdown voltage inherent in the GaN material. However, their reliability still limits their applications in today's electronic systems. The newly developed field-plated AlGaN/GaN high electron mobility transistors show improved performance due to the electric field reduction in the device channel and surface modification [2]. We report on two dimensional numerical simulations of gate-recessed and field-plated AlGaN/GaN HEMTs where all the important device parameters have been defined, the insulator thickness under the field plate is also an important design parameter to attain higher breakdown voltage, thus an improvement of the performances of HEMT devices. 1. Y. F. Wu, A. Saxler, M. Moore, R. P. Smith, S. Sheppard, P. M. Chavarkar, T. Wisleder, U. K. Mishra, and P. Parikh, IEEE Elect. Dev. Let., 25, 117 (2004) 2. K. H. Cho, Y. S. Kim, J. Lim, Y. H. Choi, M. K. Ha, Sol.Stat. Elect., 54, 405 (2010).

Which anchoring group for NiO dye-sensitized solar cells? Theoretical insights

O. V. Kontkanen[1], C. Quarti[2], D. Beljonne[2], J. Cornil[2], T. I. Hukka[3], and T. T. Rantala[1]

[1] *Laboratory of Physics, Tampere University of Technology, Tampere, Finland*
[2] *Chemistry of Novel Materials, University of Mons, Mons, Belgium*
[3] *Laboratory of Chemistry and Bioengineering, Tampere University of Technology, Tampere, Finland*

A p-type dye-sensitized solar cell, where the dye injects a hole into the semiconductor, could be combined with a typical Gratzel cell to create an efficient tandem device. However, the current p-type devices suffer from low efficiency. Here, geometries and electronic structures of trisphenylamine (TRIA) - based dyes with three different anchoring groups. The models are TRIA-CARB, -DIOL, -PYR, and NiO(100) and thet were studied within DFT. They were studied both as free and adsorbed on the semiconductor surface to investigate to gain a better understanding of the p-type devices. In particular, the electronic transitions relevant to charge transfer between the dye and the surface have been identified. The dipole moment and its effects to energy levels, and the roles of frontier orbitals and band edges in transitions have been assessed. The resulst show that PYR is the best anchoring group due to the favorable energy level alignment (HOMO of dye molecule lies 0.39 eV below the valence band maximum of semiconductor), a reasonable adsorption energy (0.57 eV), and Mulliken population analysis shows that the electron are moved from surface to dye molecule.

Dynamical screening in homogenous electron gas from Bethe-Salpeter equation

J. Koskelo[1,2], L. Reining[1,2], and M. Gatti[1,2,3]

[1] *Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, F-91128 Palaiseau, France*
[2] *European Theoretical Spectroscopy Facility (ETSF)*
[3] *Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, F-91192 Gif-sur-Yvette, France*

There are ongoing efforts to calculate properties of real materials from quantities calculated in model systems [1,2]. This can be done by designing an effective potential for a chosen observable and importing it from a model system thanks to a suitable connector. The relevant effective potential can be calculated in the model once for all in order to be imported in various real materials. This calls for a comprehensive characterisation of the model system. In this contribution, we focus on the density-density response function χ in homogenous electron gas (HEG) calculated from the Bethe-Salpeter equation (BSE). We examine the performance of the standard BSE methodology in HEG by comparing to approximations from time-dependent density-functional theory. We study a wide range of momentum transfers q and Wigner-Seitz radii r_s and look for phenomena like the appearance of the so-called "ghost exciton" [3].

[1] M. Panholzer et al, Phys. Rev. Lett. **120**, 166402 (2018).
[2] M. Vanzini et al, arXiv:1708.02450
[3] Y. Takada, Phys. Rev. B **94**, 245106 (2016).

Structure, Electronic, Vibrational Properties of Single-Layer Stanane and its Application as a Potential Gas Sensor

Vipin Kumar and Debesh R. Roy

Sardar Vallabhbhai National Institute of Technology, Department of Applied Physics, Surat (Gujarat) - INDIA

The charge transfer of toxic gas molecules (NO_2, SO_2, NH_3 and CO_2) on hexagonal chair type hydrogenated stanene has been studied in detail using density functional theory (DFT) based on an ab-initio technique. The most stable configuration, electronic properties, adsorption energies and charge transfer of these gases on stanane are systematically discussed. The band gap of the pure stanane is noticed to change 0.52 eV after interaction with gases. Moreover, the changes in the energy band gap and charge density is observed upon adsorption of NO_2, SO_2, NH_3 and CO_2 on p-type stanane based material. The results shows that the selectivity of hydrogenated stanene based gas sensors is very important to enhance their sensitivity. It is found that all the gas molecules act as charge donors in which NO_2 gas shows maximum adsorption their on the stanane surface along with maximum charge transfer. The nontrivial affectability and selectivity of stanane demonstrate that it has a potential application in the field of gas sensors and superior impetuses.

[1] Kong, Franklin, Zhou, Chapline, Peng, Cho and Dai, 2000, **287**, 622–625.
[2] J.Klinovaja and D. Loss, Phys. Rev. B, 2013, **88**, 075404.
[3] K. S. Novoselov, V. I. Fal, L. Colombo P. R. Gellert, M. G. Schwab and K. Kim, Nature, 2012, **490**, 192.

Effects of the Tamm-Dancoff approximation on the optical spectra of polythiophene molecules

Tobias Lettmann and Michael Rohlfing

Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the so called Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.
It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for some organic semiconductors [1]. Here we show the effects of the TDA on the resulting optical spectra of polythiophene molecules of different sizes. We further investigate the influence of the conjugation length of the π-system and deformations of the molecule on the applicability of the TDA.

[1] B. Baumeier et al, J. Chem. Theory Comput. **8**, 997 (2012).

Ab initio study of Silver chloride: Becquerel's photochromatic photography

Arnaud Lorin, Matteo Gatti, Lucia Reining, and Francesco Sottile

LSI, Ecole Polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France

Silver chloride has been widely used in photographic process, thanks to its sensitivity to visible light and its capacity to form latent images. It was at the heart of the works of Edmond Becquerel for the photovoltaic effect (the world's first solar cell) and the first color photographic process [1]. Its photo-reduction characteristics are reversible, which makes photochromic lenses possible. More recently, this material gained interest also as a photocatalyst [2].

In the present work, we have calculated and analyzed the optical and dielectric properties of bulk silver chloride from first principles.

We report here the calculated absorption and Electron Energy Loss spectra for a perfect crystal of Silver chloride. The calculations have been carried out within Time Dependent Density Functional Theory using the Adiabatic Local Density Approximation [3,4], as implemented in the DP code [5] and in the framework of the GW approximation and the Bethe-Salpeter equation using Abinit code [6] and Exc code [7]. We compare our results with recent experimental spectra obtained by the Centre de Recherche sur la Conservation with which we collaborate on elucidating the mechanisms that might explain the color photochromatic images of Edmond Becquerel.

[1] Edmond Becquerel in "La lumière, ses causes et ses effets", (F. Didot frères, fils et Cie (Paris)).
[2] S.Zhang et al. Chem. Eng. Journal 240, 548 (2014); J. Gou et al. J.Ind. Eng. Chem. 59, 99 (2017).
[3] E. Runge, E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984).
[4] E.K.U. Gross and W. Kohn, Phys. Rev. Lett. 55, 2850 (1985).
[5] https://etsf.polytechnique.fr/software/Ab_Initio/
[6] https://www.abinit.org/
[7] https://etsf.polytechnique.fr/exc/

Analytic understanding and control of dynamical friction

Emanuele Panizon[1], Giuseppe E. Santoro[1], Erio Tosatti[1], Gabriele Riva[2], and Nicola Manini[2]

[1] *International School for Advanced Studies, Via Bonomea 265, 34136 Trieste, Italy*
[2] *Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy*

Recent model simulations discovered unexpected nonmonotonic features in the wear-free dry phononic friction as a function of the sliding speed. Here we demonstrate that a rather straightforward application of linear-response theory, appropriate in a regime of weak slider-substrate interaction, predicts frictional one-phonon singularities which imply a nontrivial dependence of the dynamical friction force on the slider speed and/or coupling to the substrate. The explicit formula which we derive reproduces very accurately the classical atomistic simulations when available. By modifying the slider-substrate interaction the analytical understanding obtained provides a practical means to tailor and control the speed dependence of friction with substantial freedom.

Defect formation energy in LiF doped with Mg: a hybrid density functional theory study

G. Massillon-JL[1], C. S. N. Johnston[2], and J. Kohanoff[2]

[1] *Instituto de Física, Universidad Nacional Autónoma de México, 04510 Coyoacan Mexico City, México*
[2] *Atomistic Simulation Centre, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom*

LiF doped with Mg and Ti is the most commonly thermoluminescent (TL) dosimeter used to evaluate absorbed dose received by patients in clinical applications [1]. However, the relation between the energy deposited within the dosimeter sensitive volume and the TL response is not well established, mainly at low energy radiation [1]. This is due, in part, to a lack of understanding of the characteristic defects responsible for the complex structure of the observed TL glow-curve (light intensity vs temperature). In this work, formation energy [2] in LiF doped with Mg and the thermodynamic transition levels that allow evaluating the stability of the defects within the bandgap as well as the type of defect have been investigated. The hybrid-functional PBE0 [3-4], which features 25% HF exchange and the PBE semi-local functional, was selected and the implementation of the auxiliary-density-matrix method (ADMM) by Guidon et al. [5-6] was used. The calculation was performed with the DZVP-MOLOPT-SR-GTH basis sets and GTH-PBE pseudopotentials. The LiF lattice constant was 4.028Å and we used a 3 x 3 x 3 supercell containing 216 (LiF) to 217 (LiF:Mg) atoms and a 5x5x5 supercell containing 250 (Mg bulk) atoms. Preliminary results suggested that the different defect energies observed within the LiF gap are stable. And in the particular case of the Mg defect, it is a donor, i.e. an electron trap, which contrasting with previous interpretations based on phenomenological approach study. Acknowledgments We acknowledge computational support from ARCHER-UK, for which access was obtained via the UKCP consortium and funded by EPSRC grant EP/K013564/1 and from Miztli-UNAM, through grant LANCAD-UNAM-DGTIC-334. This project is partially supported by Royal Society grant NA150212 and PAPIIT-UNAM grant IN115117. References

[1] G Massillon-JL, A Cabrera-Santiago, R Minniti, M O'Brien and C Soares Phys. Med. Biol. **59** 4149 (2014)

[2] C Freysoldt, B Grabowski, T Hickel, J Neugebauer, G Kresse, A Janotti and C G Van de Walle Rev. Mod. Phys. **86** 253 (2014).

[3] J P Perdew, M Ernzerhof and K Burke J. Chem. Phys. **105** 9982 (1996)

[4] C Adamo and V Barone J. Chem. Phys. 110 **110** 6158 (1999)

[5] M Guidon, J Hutter and J VandeVondele J. Chem. Theory Comput. **5** 3010 (2009)

[6] M Guidon, J Hutter and J VandeVondele J. Chem. Theory Comput. **6** 2348 (2010)

Ab-initio TD-DFT study of linear optical properties of in-plane hetero-structures of graphene and two-dimensional hexagonal boron nitride

S. Mazzei, M. Troll, and V. Véniard

Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau CEDEX 91128

During last two decades, after the discovery of graphene, two-dimensional materials attracted a huge interest in the condensed matter physicist community. The extraordinary transport properties of this materials, as well of the atomic scale thickness and good mechanical resistance, make it a credible candidate for the realisation of next-generation electronic components. Due to this interest, several others two-dimensional materials have been synthesised after graphene, like silicene , exfoliated molybdenum disulphide and boron nitride. Combining two-dimensional semiconductors with graphene, is a good way to tune its electronic properties . In particular, in 2009, it has been demonstrated that graphene and two-dimensional boron nitride can hybridise, forming in-plane heterostructures with segregated domains. Our work takes place in this context: by mean of ab-initio Density Functional Theory, and Time-Dependent Density Functional Theory calculations, we have studied the optical properties and the band structure of several in-plane heterostructures of graphene and boron nitride. We modellised several in-plane heterostructures based on zig-zag nanoribbons with various width of C and hBN stripes. We have studied the band structure, and the evolution of the band structure and the evolution of the bandgap. Absorption spectra perpendicular and parallel to the ribbons show a strong anisotropy. We have analysed this effect in relation with the projected DOS.

Theoretical investigation on multistate system of 4,7-dihydroxy-3-methoxyflavylium : A DFT and TD-DFT study

Shaaban A. Elroby[1,2]

[1] *Chemistry Department, Faculty of Science, King Abdulaziz University, Jeddah 21589, Kingdom of Saudi Arabia*

[2] *Chemistry Department, Faculty of Science, Beni-Suef University, Beni-Suef, Egypt*

The structural transformations of 4,7-dihydroxy-3-methoxyflavylium (DMOF) have been investigated by quantum chemistry calculations. The multistate system reaches a different equilibrium involving five species for DMOF (B, QB, CT,CCT, AH+) at pH changes and light excitation. Theoretical calculations based on DFT/TD-DFT are carried out for the five studied species to understand the reversible interconverted mechanism upon pH and light. To establish this mechanism, deprotonation enthalpies, proton affinities, ionization potentials, electron affinities, and electron transfer enthalpies are calculated in gas phase. In the present work the thermal and photochemical theoretical study of DMOF described in this paper clearly shows that this compound behaves as a multistate/multifunctional system since it can exist in several forms that can be interconverted by more than one type of external stimuli such as light and pH. The calculations revealed comparable results with those obtained from the experimental data. Optimized geometrical structure was calculated with B3LYP/6-311++G** level of theory. The results indicated that all species are coplanar structures. The absorption spectra and emission of the compound were computed in gas-phase using B3LYP and CAM-B3LYP methods with 6-311++G ** basis set. The agreement between calculated and experimental wavelengths was very good at CAM-B3LYP/6-311++G** level of theory. Results indicated that interestingly only AH+ exhibit intense fluorescence bands with max at 430 nm.

Out-of-plane complexity in eumelanin protomolecules: effects of extensive stacking on optical absorption spectra of DHI-like monomers

E. Molteni[1,2,3], G. Cappellini [2,4], G. Onida[1,3], and G. Mula[2,4]

[1] *Department of Physics, Universitá degli Studi di Milano, via Celoria 16, 20133, Milan, Italy*
[2] *Department of Physics, Universitá degli Studi di Cagliari, Cittadella Universitaria di Monserrato, S.P. Monserrato-Sestu Km. 0.700, 09042 Monserrato (CA), Italy*
[3] *European Theoretical Spectroscopy Facility (ETSF)*
[4] *Istituto Officina dei Materiali (CNR-IOM) UOS Cagliari, Cittadella Universitaria di Monserrato, S.P. Monserrato-Sestu Km. 0.700, 09042 Monserrato (CA), Italy*

Eumelanin is the most common biological melanin, a photoprotective pigment displaying a broadband optical absorption spectrum with intensity monotonically increasing with frequency (*e.g.* [1]). Despite the still incomplete knowledge on the three-dimensional structure of eumelanin, due to its almost complete insolubility in all solvents and molecular heterogeneity (*e.g.* [2]), the following features are by now ascertained: 1) 5,6-dihydroxyindole (DHI), 5,6-dihydroxyindole-2-carboxylic acid (DHICA) and their various redox forms, such as indolequinone (IQ) and quinone-methide (MQ), are eumelanin basic building blocks; 2) protomolecules, resulting from the in-plane polymerization of the above-mentioned DHI-like molecules, form π-stacked arrangements of lateral size around 15-20 Å, 4-5 layer thickness and 3-4 Å interlayer distance [3,4]. The broadband and monotonic absorption spectrum of eumelanin - qualitatively different from the spectra of simple molecules such as DHI - must thus result from the complex 3D arrangement (including both out-of-plane stacking and in-plane oligomerization) of the elementary DHI-like building blocks, and/or from their chemical heterogeneity. In this work we focus on the effects of molecular stacking on the optical properties of a minimal model of eumelanin protomolecules, *i.e.* the DHI, DHICA, IQ and MQ monomers, within a first-principle approach based on plane-wave (PW) density functional theory (DFT) and time-dependent DFT (TDDFT). The use of PW DFT proves useful for describing extensive molecular stacking at a reasonable computational cost, by treating the system as periodical along the stacking direction. We analyze the effects of molecular stacking on absorption spectra, and the sensitivity of such spectra to the chemical species, the interlayer distance, the stacking geometry, the approximation inherent in our describing multi-layer stacked systems as infinite-layer ones, and the type of approximation used for the exchange-correlation kernel when calculating the dielectric function of the system. The present results provide hints on trends in the optical properties of extensive stacking forms of larger (and computationally more demanding) units, *i.e.* oligomers of DHI-like molecules.

[1] P. Meredith et al., Soft Matter **2**, 37 (2006).
[2] M. d'Ischia, et al., Angew. Chem. Int. Ed. **48**, 3914 (2009).
[3] J. I. N. Cheng et al., Pigm. Cell Res. **7**, 263 (1994).
[4] A. A. R. Watt et al., Soft Matter **5**, 3754 (2009).

Ab-Initio Study of Electrical, Optical and Mechanical Properties of Hydroxylammonium Lead Halide Perovskites (NH3OHPbX3, x=Cl, Br and I).

V. Najafi [1], S. Kimiagar[1], and M. Faghihnasiri [2]

[1] *Department of Physics, Central Tehran Branch, Islamic Azad University, Tehran, Iran*
[2] *Department of Physics, Shahrood University of Technology, Shahrood, Iran*

Nowadays, Solar cells based on organic-inorganic halide perovskites are among the most exciting topics in the field of renewable energies. In this work, through studying the cubic phase of hydroxylammonium lead halide perovskites (NH3OHPbX3, x=Cl, Br and I) structures, the effect of strain on electrical and optical properties of these materials have been investigated. Results of calculations using three approximations including PBEsol, SOC and HSE06 demonstrate that tensional strain causes the band gap increase in these structures. This tensional strain which could be equal to the thermal expansion of the material under sunlight or any mismatch with the sublayer or other reasons will change its properties and decrease its performance. Moreover, results of optical properties show that because of this dimensional expansion, the pick of adsorption diagram has blue shift and moves toward energetic photons.

Perturbation theory in a correlated basis

M. Panholzer

Johannes Kepler University Linz, Institute for Theoretical Physics, 4040 Linz, Austria

It is well known that the convergence of perturbation theory (PT) strongly depends on the starting point. For a starting point far from the true solution the convergence is poor and for states close to the exact state the lowest order yield already good results. This is seen also in many body perturbation theory. For fermionic electron gas, the starting point is usually a Slater determinant of single particle orbitals. Even for the optimal single particle orbitals the convergence is slow. A better basis set should improve convergence issues, but a strategy to go beyond the non interacting Slater determinant is not obvious. In this contribution a Jastrow correlated basis is used as the starting point for PT. This basis is constructed by combining the exited Slater determinants (particle hole exciations) with the Jastrow correlation factor of the ground state. To demonstrate the validity and accuracy of the approach the linear response of the electron gas is calculated in different approximations. The linear response is found by minimization of the action with respect to the correlated excited states. The theory is developed step by step, first neglecting exchange and optimizing only single particle hole excitations. This leads to a correlated version of RPA with a static effective interaction in contrast to the Coulomb interaction. Optimizing also 2p2h excitations improves the result further and includes dynamical effects like the double plasmon and the double peak structure at high momentum transfer[1]. As a next step, including exchange, makes the numerics more cumbersome. At the single particle hole level the correlated equivalent of time-dependent HF is obtained, but again a different effective interaction V_F has to be used in the exchange part. It is shown that V_F also appearing in the Fock energy approximates the quasi particle energy of G_0W_0 in the HEG. Thus, from the numerical point of view this is similar to BSE in the common approximation of static W and static quasi particles.

[1] M. Panholzer, M. Gatti, L. Reining, Phys. Rev. Lett. **120**, 166402 (2018)

A DFT Study of Vanadium Doped Gold Nanoalloy Clusters

Prabhat Ranjan[1] and Tanmoy Chakraborty[2]

[1] *Department of Mechatronics Engineering Manipal University Jaipur, Jaipur-303007, India*
[2] *Department of Chemistry Manipal University Jaipur, Jaipur-303007, India*

The electronic and optical properties of AunV (n=1-8) nanoalloy clusters have been investigated invoking Density Functional Theory (DFT) based descriptors. Conceptual DFT based global descriptors have been used to exhibit experimental properties qualitatively. In this report, the experimental properties of AunV (n=1-8) nanoalloy clusters are correlated in terms of DFT based descriptors viz., HOMO-LUMO energy gap, Hardness, Softness, Electronegativity, Electrophilicity Index and Dipole Moment. The doping of single vanadium atom in gold clusters enhances the stability of gold clusters and also display pronounced odd-even oscillation behaviors. The computed bond length of instant clusters are numerically close with experimental data. The linear regression analysis has been done in terms of correlation between our computed descriptors and their experimental counterparts.

Impact of Lattice Screening on Wannier-Mott Excitons

Claudia Rödl[1,2]

[1] *Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany*

[2] *European Theoretical Spectroscopy Facility (ETSF)*

Optical properties of materials are most relevant for a large variety of technological applications, ranging from photovoltaics over various spectroscopy techniques to LEDs and displays. In optical spectra, microscopic quantum many-body effects like excitons, i.e. coupled electron-hole-pair excitations, are measurable at a macroscopic scale and crucially determine the materials properties. Hence, a deep understanding of excitons constitutes an indispensable driving force for innovation in optics and optoelectronics. The state-of-the-art parameter-free theoretical description of excitons is based on the Bethe-Salpeter equation of many-body perturbation theory.

The present theoretical standard approach takes only the static electronic screening of the electron-hole-pair interaction into account. The coupling of excitons to phonons and, hence, polaronic screening contributions are omitted. However, the exciton-phonon coupling is crucial for the qualitative and quantitative understanding of exciton spectra in materials with strong polaronic effects, such as many technologically highly relevant oxides. We will tackle this problem and explore routes towards the inclusion of the polaronic screening contributions into the Bethe-Salpeter framework. As test systems, we study simple two-atomic bulk semiconductors and insulators like MgO.

Spectral dependence of the anisotropic effects of optical phonons on the optical properties of type-II Weyl semimetal WTe2

D. Soranzio[1], M. Peressi[1], R. J. Cava[2], F. Parmigiani[1,3,4], and F. Cilento[4]

[1] *Dipartimento di Fisica, Universitá degli Studi di Trieste, 34127 Trieste, Italy*
[2] *Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA*
[3] *International Faculty, University of Cologne, Albertus-Magnus-Platz, 50923 Cologne, Germany*
[4] *Elettra-Sincrotrone Trieste S.C.p.A., 34149 Basovizza, Italy*

Tungsten ditelluride (WTe2) is a transition metal dichalcogenide (TMDC), which has been receiving increasing attention due to the recent discovery of peculiar properties, such as its extremely large magnetoresistance [1] and possible topological features as a type-II Weyl semimetal [2]. To investigate the possibility to control the magnetoresistance using ultrashort laser light pulses, we studied the non-equilibrium behavior of WTe2. Using time-resolved optical spectroscopy (TR-OS), we investigated the modification of the dielectric function, induced by an 800 nm $\tilde{5}0$ fs pump pulse and measured via an ultrabroad supercontinuum probe beam. We found a highly anisotropic differential reflectivity signal for probe polarizations oriented along the a and b crystallographic axes, showing a global two-fold symmetry. Moreover, five A1 coherent optical phonons were resolved, at $\tilde{9}$ cm^{-1}, $\tilde{8}0$ cm^{-1}, $\tilde{1}17$ cm^{-1} (through single-colour measurements), $\tilde{1}33$ cm^{-1} and $\tilde{1}1$ cm^{-1}. For the two lowest energy modes, we analyzed the amplitude symmetry, temperature dependence and effects on the normal incidence reflectivity. In particular, these latest effects have been modelled invoking the modification of selected parameters of a model dielectric function and studied with ab-initio calculations. When using time- and angle-resolved photoemission spectroscopy (TR-ARPES), a large and negative photoemission intensity variation was observed just below the Fermi level along the γ direction. The time-resolved signal relaxes on a $\tilde{1}$ ps timescale, and shows no signature of coherent modulations.

[1] Ali M. N. et al., Nature 514 (2014), pp. 205–208
[2] Soluyanov A. A. et al., Nature 527 (2015), pp. 527–530

Strain engineering of lonsdaleite germanium

Jens Renè Suckert[1,2], Claudia Rödl[1,2], Jürgen Furthmüller[1,2], Friedhelm Bechstedt[1,2], and Silvana Botti[1,2]

[1] *Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany*

[2] *European Theoretical Spectroscopy Facility (ETSF)*

The integration of optoelectronics into microelectronics would allow for intra- and inter-chip communication at an attojoule/bit energy consumption. To this end, a pure silicon laser would be the ideal solution. Unfortunately, the diamond phase of silicon has an indirect band gap and though its lonsdaleite phase has a direct gap, it is optically forbidden. Lonsdaleite germanium could provide an alternative, while the relaxed structure also has an optically forbidden direct gap, this may not be the case under strain. In this work, we investigate how to manipulate the electronic structure of lonsdaleite germanium by straining the material. We employ density functional theory, using PBEsol to perform geometry optmizations and meta-GGA functionals to calculate the electronic band structure.

Structural prediction of low-energy interface reconstructions of Σ5 grain boundaries

L. Sun[1] and S. Botti[1,2]

[1] *Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany*

[2] *European Theoretical Spectroscopy Facility*

We performed $ab\ initio$ global structural predictions with the minima hopping method of interface reconstructions in three different silicon grain boundaries, $\Sigma5(012)$, $\Sigma5(031)$ and $\Sigma5(521)$. We calculated interface energies and electronic density of states. Compared with locally optimized structures, our new structures have lower total energies and significantly smaller interface energies. We observed some recurrent geometrical features of the lowest energy interfaces: Si atoms prefer to form spiral structures rather than simiple rings. Concerning the electronic properties, defect energy levels in the band gap of locally-optimized interfaces can disappear after interface reconstruction. Our investigation suggests that global structural prediction is extremly important to predict the effect on transport and optical properties of grain boundaries in semiconductors.

Hydrogenated Silicene on Ag(111): a theoretical investigation through optical excitations

A. Ugolotti[1], G. P. Brivio[1], and G. Fratesi[2]

[1] *Dipartimento di Scienza dei Materiali, Università degli Studi di Milano-Bicocca, via Cozzi 55, 20125, Milano, Italy*

[2] *Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy*

Despite the huge interest the silicene has risen as Si-based counterpart of graphene, all the extensive investigations carried onto it point to its properties being dramatically altered by the substrate onto which it is synthesized [1]. Several metal surfaces have been exploited and the Ag(111) one, which was one of the first historically considered, is no different: all studies report the loss of the desired Dirac cone due to the strength of the Si-Ag interaction affecting band structures and optical properties regardless of the specific silicene phase [2,3].

Among the several different techniques suggested to decouple the adlayer from the metal, one of the possibly simpler is the passivation through adsorption of H atoms [4]. In this direction efforts have been dedicated to understand the correct adsorption configuration in the last few years [5,6]. At the same time, new theoretical descriptions have been developed, tackling with good accuracy the excited states beyond the density functional theory (DFT) level [7,8]. The application of these new methods to complex systems would not only provide new tools of investigation, but it would also push the understanding and the efficiency of such approaches.

In this work we theoretically investigate the adsorption of silicene-based layers onto the Ag(111) surface, focusing onto the $(2\sqrt{3} \times 2\sqrt{3})R30°$ phase. We consider different H coverages, from the single atom to half-coverage and full coverage (so-called silicane). From a DFT description of the structural and electronic properties in the ground state, we construct the optical response within the independent particle approximation. We therefore address the features observed both in the absorption and reflectance spectra, showing their tight connection with the electronic properties and, finally, the role played both by the metal substrate and H atoms.

[1] Molle et al., Nature Materials **16**, 163 (2017)
[2] Sheverdyaeva et al., ACS Nano **11**, 975, 2017
[3] Cinquanta et al., Physical Review B **92**, 165427 (2015)
[4] Zhang et al., Physics Letters A **376**, 1230–1233 (2012)
[5] Qiu et al., ACSNano **9**, 11192 (2015)
[6] Wei et al., J. Mater. Chem. A **5**, 18128 (2017)
[7] Wei et al., Physical Review B **88**, 045203 (2013)
[8] Hogan et al., Physical Review B **97**, 195407 (2018)

Electronic and Transport Properties of Double-Walled Carbon Nanotubes

N. Wittemeier[1], M. Verstraete[2], L. Henrard[3], P. Lambin[3], R. Mazzarello[1], and Z. Zanolli[1]

[1] *RWTH Aachen University, Institute for Theoretical Solid State Physics, Otto-Blumenthalstraße, 52074 Aachen, Germany*
[2] *Universite de Liège, Institut de Physique, Allée du 6 aout 19, B-4000 Sart Tilman, Liège, Belgium*
[3] *Université de Namur, Départment de physique, 61 Rue de Bruxelles, B-5000 Namur*

Carbon nanotubes have 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 resistances (NDR) have 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 NDRs and identify the underlying mechanism. The multi-scale approach presented here, allows one to model multi-walled nanotubes of realistic sizes and compare with presently unexplained experimental results.

[1] S. Iijima, Nature **354**, 56-58 (1991).
[2] D. Mtsuko et al, Phys. Rev. B **91**, 195426 (2015).

Participants

The participants listed here are those who actually attended the workshop. The list has been updated after the meeting.

Austria

Martin Panholzer

Belgium

Jean-Christophe Charlier
Nicole Helbig
Pedro Melo
Gian-Marco Rignanese
Michiel van Setten
Matthieu Verstraete

Finland

Outi Kontkanen
Patrick Rinke

France

Ayoub Aouina
Claudio Attaccalite
Andrea Cucca
Gabriele D’Avino
Rubén Ferradás
Matteo Gatti
Christine Giorgetti
Jaakko Koskelo
Chenhui Li
Arnaud Lorin
Stefano Mazzei
Valerio Olevano
Lucia Reining
Francesco Sottile

Germany

Pedro Borlido
Silvana Botti
Irene Burghardt
Florian Eich
Christoph Friedrich
Hardy Gross
Tobias Lettmann
Miguel Marques
Markus Morgenstern
Claudia Rödl
Jens Renè Suckert
Lin Sun
Nicolas Tancogne-Dejean
Christian Vorwerk
Nils Wittemeier

Iran

Aidin Ahmadi
Vahid Najafi

Iraq

Shaida Kakil

Italy

Simona Achilli
Anu Baby
Gian Paolo Brivio
Marco Cazzaniga
Giulio Cerullo
Letizia Chiodo
Gianluca Colò
Cristiana Di Valentin
Guido Fratesi
Davide Grassano
Moloud Kaviani
Nicola Manini
Rocco Martinazzo
Alberto Milani
Elena Molteni

Giovanni Onida
Abhilash Ravikumar
Davide Sangalli
Davide Soranzio
Luisa Torsi
Aldo Ugolotti

Luxembourg

Pierluigi Cudazzo
Ludger Wirtz

Mexico

Guerda Massillon

Netherlands

Christiane de Morais Smith
Petra Rudolf

Spain

Alberto Castro
Zeila Zanolli

Sweden

Tomas Brage
Tuomas Rossi
Claudio Verdozzi

Switzerland

Stefano Carrazza
Matteo Cococcioni

United Kingdom

Joao Abreu
Brian Cunningham
Rex Godby
Gabriel Greene Diniz
Myrta Grüning
Samuel Poncé

United States

Giulia Galli

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Monday 10 September		
Time	Duration	Introductory lectures
14:00	**01:30**	**Steering committee**
15:30	**00:30**	**Registration & coffee**
16:00	**00:10**	**Opening**
16:10	**00:40**	**Hardy Gross: Many-body theory**
16:50	**00:40**	**Stefano Carrazza: Machine learning**
19:00	**02:00**	**Welcome drink**

Tuesday 11 September		
Time	Duration	GW and nuclear physics
09:00	**00:40**	**Patrick Rinke**
09:40	00:20	Christian Vorwerk
10:00	00:20	Brian Cunningham
10:20	**00:30**	**Coffee break**
10:50	00:20	Rex Godby
11:10	**00:45**	**ETSF general meet.**
11:55	**00:15**	**ETSF website pres.**
12:10	**02:00**	**Lunch**
14:10	**00:40**	**Gianluca Colò**
14:50	00:20	Valerio Olevano
15:10	00:20	Christoph Friedrich
15:30	00:20	Samuel Poncé
15:50	00:20	Alberto Castro
16:10	**02:00**	**Poster session (food & drinks)**

Wednesday 12 September		
Time	Duration	Ultrafast phenomena and topological insulators
09:00	**00:40**	**Giulio Cerullo**
09:40	00:20	Pedro Melo
10:00	00:20	Florian Eich
10:20	**00:30**	**Coffee break**
10:50	**00:40**	**Irene Burghardt**
11:30	00:20	Claudio Verdozzi
11:50	00:20	Tuomas Rossi
12:10	**02:00**	**Lunch**
14:10	**00:40**	**C. de Morais-Smith**
14:50	00:20	Matteo Cococcioni
15:10	00:20	N. Tancogne-Dejean
15:30	**00:30**	**Coffee break**
16:00	**00:40**	**Markus Morgenstern**
16:40	00:20	Davide Grassano
17:00	**01:30**	**Science policy (round table)**

Thursday 13 September		
Time	Duration	Data science and quantum chemistry
09:00	**00:40**	**Miguel Marques**
09:40	00:20	Michiel van Setten
10:00	00:20	Pedro Borlido
10:20	**00:30**	**Coffee break**
10:50	00:20	Matthieu Verstraete
11:10	00:20	Gabriele D'Avino
11:30	**00:40**	**Giulia Galli**
12:10	**02:00**	**Lunch**
14:10	**00:40**	**Petra Rudolf**
14:50	00:20	Zeila Zanolli
15:10	00:20	Ludger Wirtz
15:30	00:20	Pierluigi Cudazzo
15:50	00:20	Claudio Attaccalite
16:10	**03:20**	**Social program**
19:30	**06:00**	**Workshop dinner**

Friday 14 September		
Time	Duration	Quantum chemistry and transport
09:00	**00:40**	**Cristiana Di Valentin**
09:40	00:20	Alberto Milani
10:00	00:20	Anu Baby
10:20	**00:30**	**Coffee break**
10:50	**00:40**	**Rocco Martinazzo**
11:30	00:20	Simona Achilli
11:50	00:20	Nicole Helbig
12:10	00:20	Davide Sangalli
12:30	**00:15**	**Closing remarks**
12:45	**02:00**	**Lunch**