

# 16th ETSF Workshop on Electronic Excitations

**Bridging theory and experiment**



**Turin, 27-30 September 2011**

## In memoriam



Rodolfo del Sole (1944-2011) was professor of quantum theory of solids at the University of Tor Vergata, Rome (Italy), leader of the Condensed Matter Theory Group at the same university and coordinator of the Rome ETSF node. Since the early eighties he carried out pioneering research in the field of realistic calculations of optical properties of materials using first semi-empirical, then ab-initio approaches.

He was a key force in establishing and developing the ETSF, and has been a deep scientific mentor and personal friend to many members of the ETSF.

# Organizers:

Claudio Attaccalite

*Institut Neel, CNRS/UJF, NanoSTAR group – Grenoble, France*

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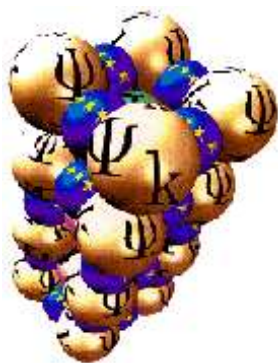
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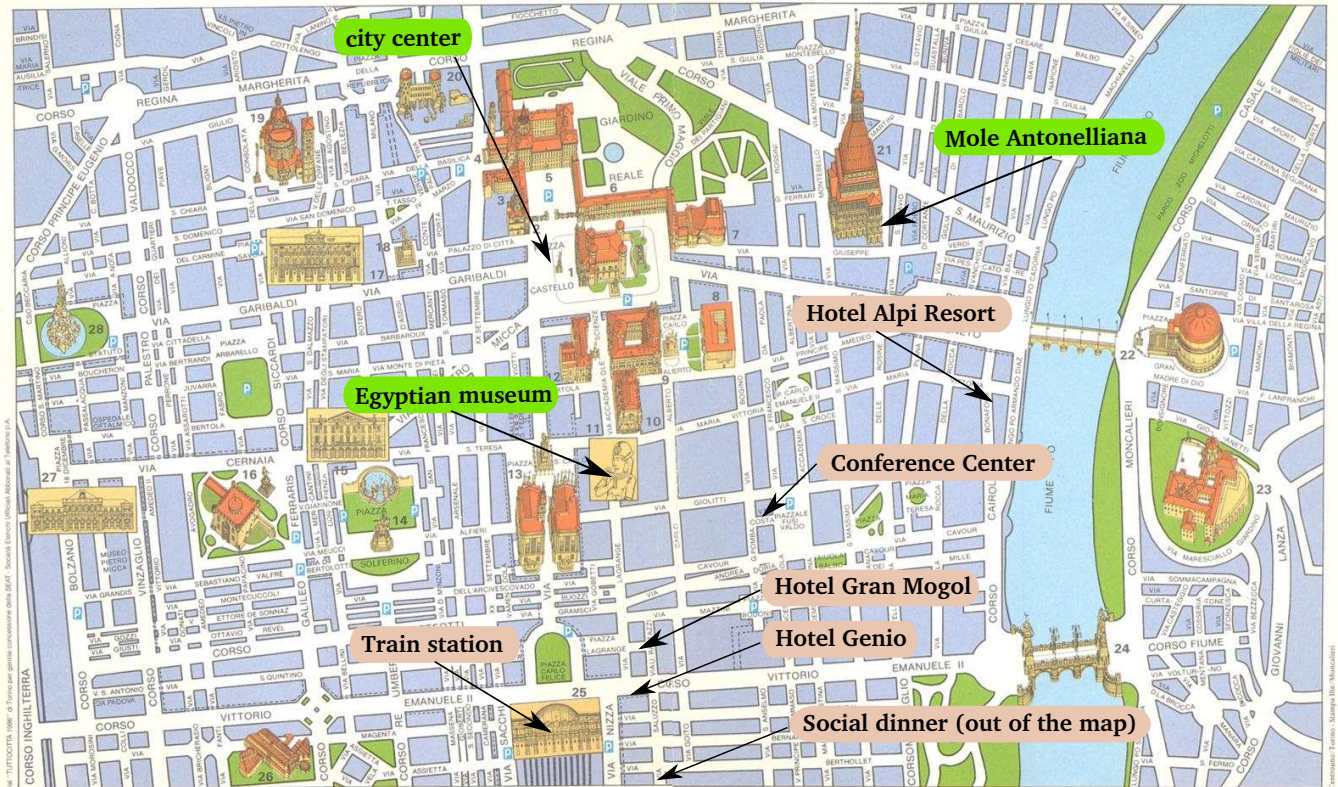
# Funding:





# Some useful information

## Map of the Center of Turin:



## Wireless connection:

Wi-Fi broadband Internet covers the whole Conference Centre. All the participants to the workshop have free access to the wireless network for the entire duration of the conference. Username and password to access the network are provided at the moment of registration. If you did not receive or lost it, please contact one of the organizers.

## Social dinner:

The social dinner will take place on the 29<sup>th</sup> September (Thursday) at 8 PM at the RISTORANTE LE DUE ISOLE (Via Saluzzo 77). The restaurant is at about 30 minutes walking distance from the conference center and can be reached by public transport.

**Tuesday 27 September**

9:00	<b>Opening</b>
9:30	Ultrafast changes of lattice symmetry at the onset of the photoinduced insulator-metal transition of VO <sub>2</sub> , <i>Julia Staehler</i>
10:00	Microscopic theory of energy dissipation and decoherence in open quantum devices, <i>Fausto Rossi</i>
10:30	Theoretical studies of ultrafast photoinduced proton-coupled electron transfer reactions, <i>A.V. Soudackov</i>
11:00	<b>Coffee Break</b>
11:30	Non-linear phenomena in time-dependent density-functional theory: What Rabi physics can teach us, <i>Johanna Fuks</i>
12:00	Size-consistency and fractional spin in Reduced Density-Matrix Functional Theory, <i>Nicole Helbig</i>
12:20	Exact exchange-correlation potentials for steady-state and time-dependent electronic systems, <i>James Ramsden</i>
12:40	<b>Lunch</b>
14:30	First-principles GW and BSE calculations for molecules of interest for organic photovoltaic applications, <i>Xavier Blase</i>
15:00	Physics with short light pulses: experiments and perspectives, <i>Franck Lépine</i>
15:30	First-principles study of the electronic and optical properties of ZnO and ZnS wurtzite nanoclusters, <i>Giuliano Mallocci</i>
15:50	Exploring the conformations, stability, and dynamics of helix-forming alanine-based polypeptides: first-principles predictions and benchmarks, <i>Mariana Rossi</i>
16:20	Ab initio electronic spectra of peptides, <i>Elena Molteni</i>
16:40	Effects of N-doping on the electronic properties of carbon atomic chains with distinct sp <sup>2</sup> graphene-like terminations, <i>G. Gueorguiev</i>
17:00	<b>Welcome Aperitif</b>
18:00	ETSF general meeting
18:30	CT reports & meetings

## Wednesday 28 September

9:00	Electronic properties of functionalized graphene <i>Alexander Gruneis</i>
9:30	The GW approximation in the FLAPW method: Applications to Oxides and Topological Insulators, <i>Stefan Blugel</i>
10:00	Satellites in Valence Photoemission Spectroscopy, <i>Matteo Guzzo</i>
10:20	<b>Coffee Break</b>
10:50	Exotic quasi-one-dimensional systems: graphene-based superlattices, <i>Lars Matthes</i>
11:20	Optical response calculations of gold alloys from first principles, <i>Deniz Kecik</i>
11:40	Strong excitons in novel two-dimensional crystals: graphane, silicane and germanane, <i>Friedhelm Bechstedt</i>
12:00	<b>Lunch + Poster Session</b>
14:20	Towards a novel approach for the calculation of many-body Green's functions, <i>Giovanna Lani</i>
14:50	Exact solution for 2-particle Green's function: an alternative to Bethe Salpeter Equation, <i>Lorenzo Sponza</i>
15:10	Strong electronic correlation in the Hydrogen chain: a variational Monte Carlo study, <i>Lorenzo Stella</i>
15:30	Properties of the screened interaction in finite systems, <i>Adrian Stan</i>
15:50	<b>Coffee Break</b>
16:20	GW/BSE Calculations of X-ray Spectra, <i>John Vinson</i>
16:50	Many-pole models of inelastic losses and satellites in x-ray spectra, <i>Joshua Kas</i>
17:10	Solids under intense ultrafast excitations: a time-dependent Bethe-Salpeter approach, <i>Andrea Marini</i>
17:30	ASE: A programmable environment for calculations with many electronic structure codes, <i>Ask Hjorth Larsen</i>
18:00	The PRACE infrastructure <i>Micael Oliveira</i>
18:20	Short GUI demos, <i>Massimo Conter, Flavio Abreu Araujo</i>

## Thursday 29 September

9:00	Kondo screening and antiscreeing in electron transport across metallic and molecular magnetic nanocontacts, <i>Erio Tosatti</i>
9:30	Electronics and Mechanics of Single Molecule Circuits, <i>L. Venkataram</i>
10:00	Spatio-Temporal description of Quantum Transport, <i>Björn Oetzel</i>
10:20	<b>Coffee Break</b>
10:50	Ab initio many-body effects in $\text{TiSe}_2$ , <i>Marco Cazzaniga</i>
11:20	Electronic Structure of Dye-Sensitized $\text{TiO}_2$ Clusters from $G_0W_0$ , <i>Noa Marom</i>
11:40	Multi-pole models for the approximation of spectral properties in GW, <i>Martin Stankovski</i>
12:10	<b>Lunch + Poster Session</b>
14:30	Probing Excited-State Potential-Energy Surfaces by Theoretical Resonance Raman Spectroscopy, <i>J. Neugebauer</i>
15:00	Electronic and mechanical properties of sp carbon atomic nanowires, <i>Nicola Manini</i>
15:20	Electron-phonon coupling in STO, <i>Bin Xu</i>
15:40	<b>Coffee Break</b>
16:10	Bootstrap approximation for the exchange-correlation kernel of time-dependent density functional theory, <i>S. Sharma</i>
16:40	Special Quasirandom Structures: application to liquid systems, <i>A. Mosca Conte</i>
17:10	A unified description of ground and excited state properties of finite systems: the self-consistent GW approach, <i>Fabio Caruso</i>
17:30	Simple preconditioning for time-dependent density-functional perturbation theory, <i>L. Lehtovaara</i>
20:00	<b>Social Dinner</b>

**Friday 30 September**

9:00	Unravelling the properties of graphene and nanotubes with Raman spectroscopy, <i>N. Bendiab</i>
9:30	NMR and EPR with Density Functional Perturbation Theory, <i>S. de Gironcoli</i>
10:00	<b>Coffee Break</b>
10:30	The polarizability and hyperpolarizability of C and BN nanotubes. A quantum-mechanical simulation, <i>Roberto Dovesi</i>
11:00	Auger Recombination and Impact Ionization from first-principles: from bulk to nanocrystals, <i>Marco Govoni</i>
11:20	Excited state properties of TiO <sub>2</sub> surfaces and nanostructures, <i>Letizia Chiodo</i>
11:40	Optical characterization of Au nanowires on Si(111) surfaces, <i>Conor Hogan</i>
12:00	<b>Lunch</b>
14:00	Phase transitions within the GW approximation, <i>Matteo Gatti</i>
14:20	Momentum Distribution and Renormalization Factor in Sodium and the Electron Gas, <i>Valerio Olevano</i>
14:40	Current issues in the description of charged defects: the case of hydrogen in amorphous silica, <i>David Waroquiers</i>
15:00	<b>Coffee Break</b>
15:30	Insights in the T-matrix approximation, <i>Pina Romaniello</i>
15:50	TDDFT dynamics for strongly correlated model systems, <i>Claudio Verdozzi</i>
16:20	<b>Closing remarks</b>
17:00	<b>Collaboration Teams Meetings</b>



## Oral Contributions

## Ultrafast changes in lattice symmetry probed by coherent phonons

Simon Wall, Daniel Wegkamp, Laura Foglia, Julia Stähler, Martin Wolf

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### Abstract

A new technique to measure ultrafast changes of the symmetry of the lattice potential initiated by a laser pulse will be presented. By monitoring the coherent optical response of our sample we indirectly detect its lattice potential. Changes to this potential modify the phonon modes of the sample and, moreover, changes of the potential *symmetry* may even lead to the vanishing of specific modes. The detection of such changes in the lattice potential symmetry is achieved by a double-pump experiment where the first pump pulse photoinduces the phase transition. This approach allows us to deduce symmetry changes on a sub-phonon-period timescale. We apply this technique to the photoinduced phase transition in VO<sub>2</sub>. A prompt change in the lattice response is observed upon crossing the phase transition threshold by the first pump pulse. This observation strongly suggests an electronically driven change in potential symmetry and will be discussed with regard to Peirls and Mott descriptions of this phase transition.

## Microscopic theory of energy dissipation and decoherence in open quantum devices

Fausto Rossi

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### Abstract

Primary goal of this talk is to provide a cohesive description of the vast field of semiconductor quantum devices, with special emphasis on basic quantum-mechanical phenomena governing the electro-optical response of new-generation nanomaterials. The talk will cover within a common language different types of optoelectronic nanodevices, including quantum-cascade laser sources and detectors, few-electron/exciton quantum devices, and semiconductor-based quantum logic gates. The distinguishing feature of the present volume is a unified microscopic treatment of quantum-transport and coherent-optics phenomena on ultra-small space- and time-scales, as well as of their semiclassical counterparts.

# Theoretical studies of ultrafast photoinduced proton-coupled electron transfer reactions

Alexander V. Soudackov and Sharon Hammes-Schiffer

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## Abstract

Photoinduced proton-coupled electron transfer (PCET) reactions play an important role in a broad range of energy conversion processes. Recent advances in time-resolved spectroscopic techniques open unique possibilities for direct probing of nonequilibrium relaxation processes in PCET systems following photoexcitation. This talk will present a theoretical formulation for modeling ultrafast dynamics of photoinduced PCET reactions in solution. In this formulation, the PCET system is described in terms of electron-proton vibronic free energy surfaces that depend on multiple collective solvent coordinates. The ultrafast nonadiabatic dynamics following photoexcitation is simulated using a surface hopping method in conjunction with coupled Langevin equations of motion describing the evolution of the solvent coordinates. The proposed methodology enables the description of concerted as well as sequential mechanisms of photoinduced PCET. It also explicitly includes effects of proton vibrational relaxation, intramolecular vibrational modes, and nonequilibrium solvent dynamics. Analysis of simulation results for a series of representative model systems, inspired by recent time-resolved spectroscopic experiments on PCET systems, provides insight into the fundamental mechanism of photoinduced PCET and reveals a complex interplay among solvent dynamics, proton vibrational relaxation, and electron and proton transfer.

# Non-linear phenomena in time-dependent density-functional theory: What Rabi physics can teach us

J.I. Fuks, N. Helbig, I.V. Tokatly, A. Rubio

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## Abstract

Through the exact solution of a two-electron singlet system interacting with a monochromatic laser we prove that all adiabatic density functionals within time-dependent density-functional theory are not able to discern between resonant and non-resonant (detuned) Rabi oscillations. This is rationalized in terms of a fictitious dynamical exchange-correlation (xc) detuning of the resonance while the laser is acting. The non-linear dynamics of the Kohn-Sham system shows the characteristic features of detuned Rabi oscillations even if the exact resonant frequency is used. We identify the source of this error in a contribution from the xc-functional to the set of non-linear equations that describes the electron dynamics in an effective two-level system. The constraint of preventing the detuning introduces a new strong condition to be satisfied by approximate xc-functionals.

# Size-consistency and fractional spin in Reduced Density-Matrix Functional Theory

N. Helbig<sup>1</sup>, N.I. Gidopoulos<sup>2</sup>, N.N. Lathiotakis<sup>3</sup>

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## Abstract

We study the behavior of different functionals of the one-body reduced density matrix (1RDM) in the dissociation of diatomic systems. We show that the error is due to an error in the description of systems with fractional  $z$ -component of the total spin and a violation of size consistency. In some cases, spin-constancy and size-inconsistency errors are partially compensating, however, without complete cancellation. We define systems with fractional spin as ensembles of integer spin states. We investigate the difference between a direct evaluation of the energy of an ensemble of integer-spin systems and a direct minimization of the energy of a fractional-spin system. It is shown that, similarly to density functional theory, the error in the dissociation of diatomic molecules is directly related to the deviation from constancy of the atomic total energies as functions of the fractional spin. An additional error in the dissociation arises from the approximations being explicit functionals of the natural orbitals and occupation numbers, instead of the one-body reduced density matrix. As a result many of the approximate functionals are not invariant under unitary transformations in the subspace of degenerate occupation numbers. One such transformation mixes the degenerate natural orbitals of identical independent subsystems, delocalizing them. Noninvariance under this transformation results in size inconsistency for some of the approximations while others avoid this pathology by favoring orbital localization.

# Exact exchange-correlation potentials for steady-state and time-dependent electronic systems

James Ramsden, Rex Godby

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## Abstract

In the Kohn-Sham formalism of Density Functional Theory and its steady-state and time-dependent variations, the interaction potential is replaced by a locally-acting effective external field. Typically this field is taken to be a local functional of the charge (and current) density; however it is known that the Kohn-Sham functional in general is not local. As such, usual approximations for the Kohn-Sham potential are missing effects present in a fully non-local calculation. We calculate the exact steady-state and time-dependent Kohn-Sham scalar and vector potentials for systems of  $N+1$  electrons governed by a non-local self-energy operator. We find that, to produce the correct charge and current densities, there is a relationship between the non-locality of the system and the strength of an intrinsic Kohn-Sham vector potential. In the absence of this vector potential, the current density of the Kohn-Sham system is typically incorrect, and the time-dependent scalar potential is forced to take extreme measures to recover the correct charge density.

# Spectroscopic properties of organic molecules within the GW and Bethe-Salpeter approach

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## Abstract

We study the quasiparticle properties, electron-phonon coupling and excitonic spectrum of organic molecules within a recently developed gaussian-basis implementation of the GW and Bethe-Salpeter formalisms (the Fiesta code). The performances of the GW approach in organic systems is tested over a large set of molecules of interest for photovoltaic applications (fullerenes, porphyrins, phtalocyanines, etc.) and DNA/RNA nucleobases [1,2], emphasizing the limits of the standard G0W0(LDA) approach in organic systems. In a second part, we study the electron-phonon coupling strength in C60 combining the GW approach together with a direct frozen-phonon technique. We show that the electron-phonon coupling potential  $V_{ep}$  calculated within the GW approach is much closer to the experimental data than the standard DFT-LDA value. Finally, charge transfer excitations in donor-acceptor systems are studied within the GW+BSE approach, showing a surprisingly good agreement with the latest TDDFT results based on variationally optimized range-separated functionals.

- [1] First-principles GW calculations for fullerenes, porphyrins, phtalocyanine, and other molecules of interest for organic photovoltaic applications, X. Blase, C. Attaccalite, and V. Olevano, Phys. Rev. B 83, 115103 (2011).
- [2] First-principles GW calculations for DNA and RNA nucleobases, Carina Faber, Claudio Attaccalite, V. Olevano, E. Runge, and X. Blase, Phys. Rev. B 83, 115123 (2011).



## Physics with short light pulses: experiments and perspectives

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### Abstract

The development of ultrashort and intense pulses technology has allowed the emergence of ultrafast science in which the motion of electrons and nuclei is probed at their intrinsic timescale. The most recent developments gave birth to short XUV, attosecond pulse sources and free electron lasers. In this talk, we will present recent experimental results performed on gas phase species. We will emphasize new possibilities offered by the modern light sources and the questions that these results have raised that require theoretical investigations.

## First-principles study of the electronic and optical properties of ZnO and ZnS wurtzite nanoclusters

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### Abstract

Zinc oxide (ZnO) and zinc sulphide (ZnS) nanostructures have emerged in recent years as promising candidates in the development of nanoscale electronic and photonic devices. Theoretical studies on the properties of nanosized wurtzite ZnO and ZnS are rather scarce and their electronic and optical properties are largely unknown to date. As a part of a more general theoretical effort aimed at the multiscale modelling of nanohybrids for photovoltaics, we computed size-dependent electronic and optical properties of ZnO and ZnS nanoclusters with wurtzite structure, using Density Functional Theory (DFT), Time-Dependent DFT (TD-DFT) and Many Body Perturbation Theory methods. We discuss general trends for binding energy, ionization energy and electron affinity, quasiparticle gap, excitonic effects, and optical absorption spectra as a function of cluster size and wire diameter. A comparison between TD-DFT and Many Body theories shows for both materials a general good agreement for the optical absorption spectra of this class of nanocrystals.

# Exploring the conformations, stability, and dynamics of helix-forming alanine-based polypeptides: first-principles predictions and benchmarks

Mariana Rossi, Volker Blum, and Matthias Scheffler

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## Abstract

Accurate theoretical predictions for peptides and proteins (structure, dynamics, function) require an accurate, verified description of the underlying potential energy surface (PES). However, a completely trustworthy treatment with the accuracy of quantum-mechanics first-principles methods, that is affordable even for moderately sized systems (few hundred atoms) is arguably not yet settled. We here show experiment-theory benchmark studies on the structure of the helix-forming alanine-based peptides Ac-Ala<sub>n</sub>-LysH<sup>+</sup>,  $n=4-15$ , in the gas phase. We employ density-functional theory with a (density-dependent) C<sub>6</sub>[n]/R<sup>6</sup> correction [1] added to the PBE exchange-correlation functional (PBE+vdW). For  $n=4-8$  we perform an extensive conformational search of more than 10<sup>5</sup> conformers, starting from a pre-screening using a force-field, followed by relaxation of thousands of conformers using the PBE+vdW functional. The capabilities and limitations of the search methodology are discussed. The onset of  $\alpha$ -helical structure is predicted at  $n=8$ , in agreement with experiment [2]. Vibrational entropy is found to play an important role on the stabilization of  $\alpha$ -helices at finite temperatures. The low (free-)energy structures found for  $n=5, 10, 15$  show a good agreement with structure-sensitive experimental IR spectra at room temperature, especially when the dynamics of the molecule and anharmonic contributions to the vibrations are taken into account [3]. Finally, we provide benchmark data for intramolecular energy differences using perturbation theory [EX+cRPA and methods based on it, using orbitals from PBE and PBE0 hybrid DFT]. We find a significant dependence on the starting point.

[1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. **102**, 073005 (2009);

[2] M. Kohtani and M. Jarrold, J. Am. Chem. Soc. **126**, 8454 (2004);

[3] M. Rossi *et. al*, J. Phys. Chem. Lett. **1**, 3465 (2010).

## Ab initio electronic spectra of peptides

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### Abstract

We present ab-initio results on the electronic spectra of a peptide corresponding to the (83-92) fragment of HIV-1 protease, a molecule of biological interest. This study is part of a project aimed at the study of circular dichroism (CD), a useful technique able to discriminate between different secondary structures of biomolecules. Since circular dichroism is due to the difference in molar extinction between left and right circularly polarized light by chiral media, it is related to absorption itself. Therefore, our study started from the calculation of optical spectra. The investigated system (a 175-atoms peptide) displays interesting features, such as charge transfer excitations, typical of "large" molecules, and resulting from specific properties and spatial localization of wavefunctions. This behaviour is therefore identifiable and understandable only through ab-initio electronic structure calculations, which we do on geometrical structures obtained by classical molecular dynamics simulations.

## Effects of N-doping on the electronic properties of carbon atomic chains with distinct sp<sup>2</sup> graphene-like terminations

Renato B. dos Santos<sup>1</sup>, R. Rivelino<sup>1</sup>, F. de Brito Mota<sup>1</sup>, G. K. Gueorguiev<sup>2</sup>

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### Abstract

Carbon nanostructures consisting of corannulene/coronene-like pieces connected by atomic chains and doped with nitrogen atoms have been addressed by carrying out first-principles calculations within the framework of the spin-polarized density functional theory. The terminations were chosen as two chemically synthesizable (i.e., experimentally viable) molecules. Our results show that the conformation, charge distributions, and spin states are significantly influenced by the nitrogen incorporation in comparison to these characteristics of similar pure carbon structures. Higher concentration of incorporated nitrogen leads to a smaller HOMO-LUMO gap and different conductive states near the Fermi level. In turn, the different location of the N incorporation sites allows switching on and off the pi-electron magnetism in these systems. Our findings indicate that by controllable N doping one can tune the conducting channel of carbon chains connected to sp<sup>2</sup> terminations, thus obtaining low band-gap nano-units.

## Electronic properties of functionalized graphene

Alexander Grueneis and Danny Haberer

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### Abstract

Regarding the device applications of graphene, chemical functionalization is one of the key strategies to tailor its electronic properties. We have carried out functionalization of chemical vapour deposition (CVD) grown graphene monolayers with alkali, nitrogen and hydrogen atoms [1,2]. This enables us to tune the energy bandgap as well as the electron concentration of graphene independently. Angle-resolved photoemission spectroscopy at synchrotron light sources is employed to directly measure the spectral function which gives us full access to the electron-phonon coupling and their dependence on doping level, wavevector direction and impurities. For fully hydrogenated graphene we observe a maximum coverage of 25 at. % in agreement with MD simulations of the hydrogenation kinetics which predicts a para-type chemisorption pattern [3]. Furthermore, a metal to insulator transition in graphene is discussed in terms of band insulator versus electron localization.

[1] Danny Haberer et al. Nano Lett. 2010, 10, 3360–3366.

[2] Danny Haberer et al. Phys. Rev. B 2011, 83, 165433.

[3] Danny Haberer et al. Advanced Materials in press 2011

# The GW approximation in the FLAPW method: Applications to Oxides and Topological Insulators

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## Abstract

Modern spintronics and quantum information explores a large spectrum of materials that act as oxide barriers or exhibit interesting magnetic and spin properties. Low energy excitations play an important role. The GW approximation for the electronic self-energy yields quasiparticle band structures in very good agreement with experiment. Most implementations so far are based on the pseudopotential approach, which limits their range of practicable applicability. We have developed an implementation (SPEX, <http://www.flapw.de/spex/>) [1] within the full-potential linearized augmented-plane-wave (FLAPW) method, which treats core and valence electrons on an equal footing. Within this method a large variety of materials can be treated, including d- and f-electron systems, oxides and magnetic systems. Our implementation employs a mixed product basis for the representation of basis-function products in the interstitial and muffin-tin regions. The self-energy can be evaluated either by an analytic continuation from the imaginary frequency axis or directly by a contour integration. A basis transformation to the eigenfunctions of the Coulomb potential allows a reduction of the basis-set size, thus leading to a considerable speed up in computation time. The code can also deal with spinor wave functions that result from a spin-orbit coupling term in the Hamiltonian. First results for mercury chalcogenide compounds whose heterostructures yielded the first two-dimensional topological insulators show a considerable quantitative improvement of the inverted band structures, in particular for the negative band gap, but also for the spin-orbit splitting. In this talk we focus on results of materials whose physics is determined by the spin-orbit interaction and on oxide materials in particular perovskites. The convergence of GW calculations with respect to the number of unoccupied states is discussed for ZnO, that developed to a prominent example [2,3] with respect to this issue.

Acknowledgement: The work was performed in collaboration with Andreas Gierlich, Mathias C.T.D. Müller, and Christoph Friedrich from Jülich and the Ferdi Aryasetiawan group in Chiba (Japan) in particular Rei Sakuma. Financial support from the Deutsche Forschungsgemeinschaft through the Priority Programme 1145 is gratefully acknowledged.

[1] C. Friedrich, S. Blügel, and A. Schindlmayr, Phys. Rev. B 81, 125102 (2010).

[2] B.-C. Shih, Y. Xue, P. Zhang, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 105, 146401 (2010)

[3] C. Friedrich, M. C. Müller, and S. Blügel, Phys. Rev. B 83, 081101 (2011).



## Satellites in Valence Photoemission Spectroscopy

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### Abstract

The  $GW$  method[1] has shown to be very successful in the description of photoemission spectra in a variety of systems. In particular,  $GW$  is known to give good quasiparticle properties like band-gaps. However, it has shown some limitations regarding the description of other more complex spectral features like satellites. Satellite peaks in photoemission come from higher-order excitations, e.g. plasmons, and are still poorly studied in real materials. In  $GW$  the spectral function  $A(\omega)$  can describe additional features beside the quasiparticle peaks, but these satellites are known to be too weak and too low in energy, as it appears from calculations on the Homogeneous Electron Gas[2] and on some real materials[3]. It is not clear whether self-consistency could improve the results. We have thoroughly studied the  $GW$  spectral function of bulk Si as a test case, trying to understand the flaws of  $GW$  in this respect. Here we compare the theory with new XPS experimental data. These data clearly show multiple plasmon replicas in the photoemission spectrum which are not reproducible within  $GW$ . The cumulant expansion (CE) ansatz for the Green's function, very popular in core-level spectroscopies, has been able to describe satellites correctly within this framework. In the case of valence spectroscopy much less data are available and results are not conclusive[3]. By means of rigorous approximations on the exact 1-particle Green's function's differential equation, we obtain an exponential solution, very close to the CE. This solution is applied to the case of bulk Si. The effect of photon cross sections, secondary electrons, extrinsic losses and interference between intrinsic and extrinsic are included. We show that our approach gives excellent agreement with experiment and discuss how to improve this result even further.

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# Exotic quasi-one-dimensional systems: graphene-based superlattices

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## Abstract

Electrons in solids that are constrained in one or more spatial dimensions may exhibit new interesting properties compared to common three dimensional bulk materials. In 1963, Luttinger studied a gas of interacting electrons in one dimension – today known as the Luttinger model – which exhibits collective charge- and spin-density waves as the elementary excitations of the system. Moreover, these waves propagate independently and with different velocities through the system whereby spin and charge of the particles are separated. As a consequence, the model of a Fermi-liquid with the well established quasi-particles carrying spin and charge breaks down in one dimension and must be described within the framework of a Luttinger liquid. Here, we give an introduction of the Luttinger model and its solution. Furthermore, a brief overview of its physical properties that can be derived by means of Greens functions is presented and discussed. Besides the model we will focus on quasi-1D graphene superlattices [1] which allow a systematic tuning of the band structure. An impressive example for such modifications has been predicted by recent Kronig-Penney-type calculations [1] for a single graphene layer subjected to a 1D periodic potential where a rather counterintuitive anisotropic renormalization of the Fermi velocity due to the Klein paradox is expected. We present first-principles DFT calculations of graphene superlattices using the VASP code. The influence of the periodic external potential on the charge-carrier redistribution and corresponding screening effects is investigated in detail. The resulting consequences for the ab-initio band structure including anisotropy effects are studied and compared with analytical calculations based on the Dirac Hamiltonian. Deviations due to self-consistent inclusion of screening effects and nonlinear dispersions are analyzed. Finally, consequences for the practical realization of graphene superlattices with 1D transport properties are discussed [2]. We will also report about approaches for the realization of real graphene-based superlattices including graphene-based heterostructures for the implementation of an intrinsic superlattice potential without the need of external fields.

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# Optical response calculations of gold alloys from first principles

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## Abstract

The optical response of pure FCC gold and gold-based alloys is investigated in the framework of density functional theory (DFT). We compare the performance of local, semilocal, and nonlocal (hybrid HSE06) exchange-correlation (XC) functionals. The hybrid XC functionals are known to increase the bandwidth, however the physics behind this improvement is still not completely understood. Alongside, quasiparticle corrections to the DFT eigenvalues in the GW approach were shown to perform well, an example being the improvement to the discrepancies in the bandstructures of Cu and Ag [1,2]. The comparison between methods such as standard-DFT, hybrid functionals and many-body perturbation theory (GW approximation), is taken into account from the aspect of accuracy of the optical properties of Au. Relations of the optical spectra to the bandstructure are discussed profoundly. We consider a series of ordered intermetallic phases such as AuAl<sub>2</sub> with substitutions of Pt instead of Au. The calculated bandstructures and optical response give us insight into the nature of interband transitions, the optical absorption edge; hence the major changes in the reflectivity. Particular attention is paid to how well the comparison is to the experiments (with an emphasis on the effect of alloying on the color). It is found that the rapid drop-off in the reflectivity of gold, calculated within the local density approximation (LDA) and generalized gradient approximation (GGA) is far off from experiments by up to 100 nm to the longer wavelength limit. On the other hand, the HSE06 approach produces a shift to the shorter wavelength limit with a slight overcorrection. Finally, standard-DFT calculations for the intermetallic alloys [(Au-Pt)Al<sub>2</sub>] point out to a nice trend in the reflectivity curves in terms of slope and dip positions, going from one composition to the other.

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## Strong excitons in novel two-dimensional crystals: graphane, silicane and germanane

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### Abstract

Excitons in sheet crystals are very poorly understood till now. Only graphane, the hydrogenated graphene, is known to exhibit excitonic features in the UV spectral region. We show by first-principles calculations that due to depressed screening and enhanced confinement, strong excitonic resonances appear in visible light/near UV spectra of hydrogenated Si and Ge layers. Their large exciton binding energies and oscillator strengths make them extremely promising for observation of novel physical effects and application in optoelectronic devices on the nanoscale.

## Towards a novel approach for the calculation of many-body Green's functions

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### Abstract

In this work, an alternative route to the calculation of the one particle Green's function (GF) has been explored. Its aim is to remedy to the shortcomings of other many-body approaches, e.g. the GW approximation (GWA), in treating strong effects of correlation in solids. The idea consists of solving a set of non-linear, differential, functional equations, which are pivotal to many-body perturbation theory. In a first instance, a so called 1-point model is employed (only one value for each time, spin, spatial variable is retained) and the set of equations reduces to a single algebraic equation, for which an explicit exact solution is obtained. The solution is used as a benchmark tool to analyze the performances of established many-body methods (e.g. different GW flavours), moreover alternative approximations are devised and for the most promising ones the generalization to their full functional form is discussed. The last part of the work deals with the generalization of the approach beyond the 1-point framework. First the frequency dependence of the GF is restored (while still retaining the 1-point approximation for the space and spin variables) and the set of equations is solved. It is shown that in such framework it is possible to recover the so-called cumulant expansion for the GF, an approximation which is beyond GW and provides accurate spectral functions for photo emission experiments. Finally, through an ansatz, a family of solutions for the equations in their full functional form is obtained and routes to approximate the physical one, far beyond the present state-of-the-art, are proposed.

# Exact solution for two-particle Green's function: an alternative to Bethe Salpeter Equation

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## Abstract

In optics, absorption spectra are computed via the evaluation of the polarizability of the material who plays a key-role in optical phenomena. This quantity is given by the differentiation of the Green's function  $G$  with respect to an external (perturbing) potential  $U$ . Recently a 1-particle Green's function ( $G_1$ ) has been derived as exact solution to a differential functional equation. In this derivation the screened Coulomb interaction can be modelled to account for different contribution, as eg plasmon satellites[1]. Aim of this work is to follow the same approach and strategy of the derivation [1] to get to an expression for the polarizability that allows to describe accurately dynamical effects in optical spectra, as for example, exciton-exciton interactions or multiple exciton generation (MEG)[2].

[1] M.Guzzo et al, to be published

[2] see for instance Kheifets et al. , Phys Rev. B 68 (2003), 233205

# Low energy physics of the Hydrogen chain beyond the Hubbard model

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## Abstract

Strong electronic correlation is not properly modeled by Density Functional Theory in its current local or semi-local approximations, while explicit many-body techniques, e.g., Quantum Monte Carlo methods, have been mostly applied to semiempirical models of strongly correlated solids. Here we report the first, fully ab initio Variational Monte Carlo study of the homogeneous Hydrogen chain, a system which provides the simplest example of strong electronic correlation in low dimensions. In particular—and at variance with the common belief that the one-dimensional Hubbard model accurately describes the low energy physics of the Hydrogen chain—we find for small interatomic distances a clear deviation from the Hubbard model predictions, while for large interatomic distances good agreement with the model is retrieved. The origin of this deviation, the limitation of the simple Hubbard model, and the role of the inhomogeneous part of the electron correlation are finally discussed.



## Properties of the screened interaction in finite systems

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### Abstract

We perform ground state and time-dependent GW calculations on finite systems, i.e., atoms, molecules and molecular chains described by model hamiltonians, and we investigate the properties of the screened interaction in terms of self-consistency. With the aid of two computational schemes, we study the convergence of the screened interaction and observables like total energies, in the ground state. Since we use the finite temperature formalism and calculate the Green function on the imaginary time axis, this allows for a simple extension to nonequilibrium systems. Starting from a ground state, we perturb the systems both with constant fields and delta-kicks and we study the spatial and temporal properties of the screened interaction - and also of the time-dependent self-consistent solutions in general - for different systems.

## GW/BSE Calculations of X-ray Spectra

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### Abstract

We present calculations of x-ray spectra, including x-ray absorption (XAS) and nonresonant inelastic x-ray scattering (NRIXS), based on a many-body perturbation theory, GW/Bethe-Salpeter Equation, approach. Ab-initio wave functions are calculated using the plane-wave, pseudopotential code ABINIT and quasi-particle self-energy corrections are added using an approximate GW correction. Our approach builds in spin-orbit interactions, intra-atomic Coulomb integrals, core-hole screening, and band-structure effects, thus also accounting for multiplet effects. Results will be presented for a variety of materials including 3d transition metal L23-edges and the O K-edge of ice.

# Many-pole models of inelastic losses and satellites in x-ray spectra

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## Abstract

Calculations of inelastic losses in x-ray absorption spectra (XAS) and other core-spectroscopies typically employ semi-empirical or simplified models, such as the plasmon-pole self-energy and the quasi-particle approximation. Here we discuss an efficient approach for calculating inelastic losses due to intrinsic and extrinsic inelastic losses and the interference between them using a quasi-boson model with many-pole representation [1]. This approach includes both quasiparticle effects and the satellite structure in the spectral function via a cumulant expansion. This method is based on first principles calculations of the dielectric function in the long-wavelength limit and an approximate excitation dispersion relation, which is then fit to a pole model with about 100 poles. This method is compared with an alternative, more precise approach based on a Lanczos algorithm for the inverse of the dielectric matrix [2]. Both approaches yield approximations for the complex GW self-energies and for the satellite terms in the spectral function. An extension of the approach for treating charge-transfer satellites in correlated systems is also discussed. The approaches are illustrated with applications to XAS spectra of several complex systems. \*Supported by DOE Grant DE-FG02-97ER45623 and facilitated by the DOE CMCSN.

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# Solids under intense ultrafast excitations: a time-dependent Bethe-Salpeter approach

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## Abstract

Many-body effects are known to play a crucial role in the electronic and optical properties of solids and nano-structures. Nevertheless the majority of theoretical and numerical approaches able to capture the influence of Coulomb correlations are restricted to the linear response regime. In this talk we introduce a novel approach based on a real-time solution of the electronic dynamics. The proposed approach, based on the Baym-Kadanoff equations of Non-Equilibrium Green's Function Theory, reduces to the well-known Bethe-Salpeter equation in the linear limit regime and it makes possible, at the same time, to investigate correlation effects in nonlinear phenomena. We show the flexibility and numerical stability of the proposed approach by calculating the dielectric constants and the effect of a strong pulse excitation in paradigmatic bulk materials.

## ASE: A programmable environment for calculations with many electronic structure codes

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### Abstract

I will present the Atomic Simulation Environment (ASE), which is a free open-source software package for atomistic calculations. ASE contains utilities for setting up structures and algorithms for tasks such as structure optimization and molecular dynamics. ASE specifies an interface through which total energy and force calculations can be performed. Through this interface, many different electronic structure or empirical codes are made available as pluggable calculator objects. The separation of individual electronic structure calculations from enclosing algorithms increases the portability of calculations between different codes. Calculations with ASE are written as Python scripts, a highly programmable alternative to traditional text input files. I will demonstrate how the scripting interface can be used to set up and run calculations.

## Short AbinitGUI demonstration.

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### Abstract

AbinitGUI is a new project inside the Abinit project with the aim of making Abinit easier to use by taking in charge some mechanical and boring common operations. This presentation is a tutorial-like demonstration of the software where the main features are explained.

# Kondo screening and antiscreeing in electron transport across metallic and molecular magnetic nanocontacts

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## Abstract

Magnetism at nanocontacts involves deep physics. It also provides an ideal means to control and modify conductance through external fields. Our current aim is to compute the effect of magnetic impurities on the ballistic conductance of metallic nanocontacts starting from first principles. This is made possible by a technique recently developed in our group. [1] The method proceeds via a conventional density functional calculation of spin and symmetry dependent electron scattering phase shifts, followed by the subsequent numerical renormalization group solution of Anderson models - whose ingredients and parameters are optimized so as to reproduce these phase shifts. We are applying this method to investigate the Kondo zero bias anomalies that would be caused by adsorbed Co and Fe adatoms in the ballistic conductance of perfect metallic (4,4) and (8,8) single wall carbon nanotubes, ideally connected to leads at the two ends. A large difference emerges between external and internal impurity absorption geometry. [2] Another interesting problem is conduction across contacted magnetic molecules. Unlike ordinary molecules that as a rule conduct very poorly, a magnetic molecule will as a rule conduct very well at sufficiently low temperature, thanks to the Kondo effect. The emergence of ferromagnetic Kondo effects at nanocontacts [3] is yet another very exciting line. Current work is aimed at identifying magnetic molecular nanocontacts that may develop ferro Kondo effects and related conductance anomalies.

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[2] P. Baruselli et al., Physica E (2011), doi:10.1016/j.physe.2011.05.005; and to be published.

[3] P. Gentile et al, EPL, 87 , 27014 (2009)

(\*) In collaboration with P. Baruselli, S. Costamagna, M. Fabrizio, R. Requist, A. Smogunov

# Electronics and Mechanics of Single Molecule Circuits

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## Abstract

Understanding and controlling electron transfer across metal/organic interfaces is of critical importance to the field of organic electronics and photovoltaics. Single molecule devices offer an ideal test bed for probing charge transfer details at these interfaces. Results from these single-molecule measurements can be directly related directly theoretical models, unlike measurements at the ensemble level. The ability to fabricate single molecule devices and probe electron transfer reliably and reproducibly has enabled us to study and model transport through them. In this talk, I will review the scanning tunneling microscope break-junction technique we use to measure electronic transport through single molecule junctions. I will discuss our measurements using novel metal-molecule link chemistries, including amines, phosphines[1] and results from recent work using tri-methyl tin linkers, which yield direct Au-C coupled single molecule junctions[2]. I will show how the intrinsic molecular properties influence measured single molecule conductance and bond rupture forces[3]. Finally, I will show how a mechanically controlled binary single molecule switch can be created using bipyridine molecules[4].

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## Spatio-Temporal description of Quantum Transport

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### Abstract

We present a numerical method for the calculation of time-dependent transport properties of non-periodic systems connected to electron reservoirs. The approach is based on the solution of the time-dependent Schrödinger equation combined with the emitting boundary conditions using plane waves as modeling of the leads. Using the approach we are able to simulate the temporal evolution of wave packets through potential barriers. Within the quasi-stationary limit the method can be associated with the Landauer Formalism. Transmission functions are calculated directly from the transmitted and reflected currents for the insertion of a single plane wave. Beyond the calculation of transmission functions the approach is also capable of field-dependent transport properties such as current voltage characteristics. Those can be calculated independently of the transmission functions including by direct treatment of time-dependent potentials and electrical fields, in contrast to the Landauer approach. The success of the method is demonstrated by 1D-model calculations for single and double barriers including modifications due to applied electrical fields.

## Ab initio many-body effects in $\text{TiSe}_2$

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### Abstract

$\text{TiSe}_2$  is a non-conventional Charge-Density-Wave material, whose ground state is believed to be a coherent exciton condensate called the Excitonic Insulator. DFT calculations give a metallic ground state with top-of-valence and bottom-of-conduction too much overlapping. On the contrary experiments predict this system to be a semi-metal or an indirect gap semiconductor, with a very small gap/overlap. More refined ab initio GW calculations predict this system to be a semiconductor with a 0.2 eV gap. In addition they provide a renormalization of the band structure around the  $\Gamma$  point, arising a mexican-hat dispersion as predicted by Kohn in an excitonic insulator. We will present and discuss excited state properties comparing calculations with ARPES, STS, and EELS measurements.

# Electronic Structure of Dye-Sensitized TiO<sub>2</sub> Clusters from G<sub>0</sub>W<sub>0</sub>

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## Abstract

The development of new types of solar cells is driven by the need for clean and sustainable energy. In this respect dye sensitized solar cells (DSC) are considered as a promising route for departing from the traditional solid state cells. The physical insight provided by computational modeling may help develop improved DSCs. To this end it is important to obtain an accurate description of the electronic structure, including the fundamental gaps and level alignment at the dye-TiO<sub>2</sub> interface. This requires a treatment beyond ground-state density functional theory (DFT). In this talk I will present a many-body perturbation theory study, within the G<sub>0</sub>W<sub>0</sub> approximation, of two of the crystalline phases of dye-sensitized TiO<sub>2</sub> clusters, reported by Benedict and Coppens [J Am Chem Soc 132 (9), 2938 (2010)]. I will demonstrate that even when DFT gives a good description of the valence spectrum and a qualitatively correct picture of the electronic structure of the dye-TiO<sub>2</sub> interface, G<sub>0</sub>W<sub>0</sub> calculations yield more valuable quantitative information regarding the fundamental gaps and level alignment. In addition, I will discuss the issues pertaining to G<sub>0</sub>W<sub>0</sub> calculations, namely: (i) convergence with respect to the number of basis functions, (ii) dependence on the mean field starting point, and (iii) the validity of the assumption that the DFT wave-function is a good approximation to the quasi-particle wave-function. I will show how these issues are manifested for dye molecules and for dye-sensitized TiO<sub>2</sub> clusters.

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2. N. Marom, X. Ren, J. R. Chelikowsky, and L. Kronik "Electronic Structure of Copper Phthalocyanine from G<sub>0</sub>W<sub>0</sub> Calculations", to be published

## The $G^0W^0$ band gap of ZnO: effects of plasmon-pole models

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### Abstract

We have performed carefully converged calculations for the band gap of ZnO within Many-Body Perturbation Theory ( $G^0W^0$  approximation). The results obtained using four different well-established plasmon-pole models are compared with those of explicit calculations without such models (the contour-deformation approach). This comparison shows that surprisingly, plasmon-pole models depending on the  $f$ -sum rule gives *less* precise results. In particular, it confirms that the band gap of ZnO is underestimated in the  $G^0W^0$  approach as compared to experiment, contrary to the recent claim of Shih et al. [Phys. Rev. Lett. **105**, 146401 (2010)].

## Probing Excited-State Potential-Energy Surfaces by Theoretical Resonance Raman Spectroscopy

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### Abstract

Probing Excited-State Potential-Energy Surfaces by Theoretical Resonance Raman Spectroscopy Resonance Raman spectroscopy is a versatile tool for the structural characterization of molecular systems as well as for investigations on photophysical and photochemical processes. One of its main advantages is the fact that the resonance can be tuned to excited states of particular chromophore groups, so that vibrations of those groups can selectively be enhanced. This is of particular importance for investigations on biomolecular systems. In this talk, we present our recent methodological advancements concerning theoretical approaches that mimic this experimentally observed selectivity [1] as well as extensions to vibrational resonance Raman optical activity, which can be used to probe chiral molecules [2]. We present applications of theoretical resonance Raman spectroscopy to the structural characterization of the carotenoid spheroidene in the photosynthetic reaction center of purple bacteria [3], where it can help to solve a long-standing riddle, and to the investigation of the first photoexcitation steps in a model for artificial photosynthesis [4].

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## Electronic and mechanical properties of sp carbon atomic nanowires

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### Abstract

Ab-initio calculations within Density Functional Theory combined with experimental Raman and infrared spectroscopy on (i) cluster-beam deposited pure carbon films and (ii) dinaphthylpolyynes provide a consistent picture of sp-carbon chains stabilized by sp<sup>3</sup> or sp<sup>2</sup> terminations. The latter are sensitive to torsional strain: this unexplored effect promises exciting applications since it allows one to modify the conductive states near the Fermi level and to switch on and off the on-chain pi-electron magnetism. sp-carbon chains are also interesting for their mechanical properties: high longitudinal versus very soft bending stiffness.

## Electron-phonon coupling in STO

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### Abstract

Within Boltzmann's transport theory, we have implemented a first-principles algorithm in ABINIT to calculate properties of solids that are related to the electron-phonon interactions. As an application, we studied the transport properties and superconductivity in SrTiO<sub>3</sub> (STO). Comparing with the measured electrical conductivity of doped STO, our prediction yields significant overestimation for highly doped case, while good agreement is achieved for intrinsic STO. The discrepancy may be attributed to the existing defects and impurities in the experimental samples. Our calculated relaxation time of electron decreases significantly with increase of temperature, and the ratio between conductivity and relaxation time is consistent with the results from the BoltzTraP approach. We also calculated the critical temperature of superconductivity for STO. By fitting to the experimental T<sub>c</sub>, we found the Coulomb repulsion parameter increases almost linearly with the increasing concentration of conduction electrons.

## Bootstrap approximation for the exchange-correlation kernel of time-dependent density functional theory

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### Abstract

A new parameter-free approximation for the exchange-correlation kernel  $f_{xc}$  of time-dependent density functional theory is proposed. This kernel is expressed as an algorithm in which the exact Dyson equation for the response as well as a further approximate condition are solved together self-consistently leading to a simple parameter-free kernel. We apply this to the calculation of optical spectra for various small bandgap (Ge, Si, GaAs, AlN, TiO<sub>2</sub>, SiC), large bandgap (C, LiF, Ar, Ne) and magnetic (NiO) insulators. The calculated spectra are in very good agreement with experiment for this diverse set of materials, highlighting the universal applicability of the new kernel.

# Special Quasirandom Structures: application to liquid systems

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## Abstract

Among the methods used to calculate excited state properties of materials, those based on the interacting two-particle Green's function within the first-principles GW-Bethe-Salpeter equation formalism [1-5] are among the most promising. However, simulations based on this methodology, require a considerable computational effort and are almost prohibitive for systems with large unit cells, such as disordered systems and liquids. One possible solution is to replace one huge unit cell by several configurations with a much lower number of atoms/molecules and to average the results obtained for these configurations. This approach led to good results [6] for liquid water and opened the way to the ab-initio calculation of other disordered systems. However it remains a lengthy and laborious task. In 1990, Zunger and coworkers [7] proposed a method, called Special Quasirandom Structures, to avoid to look upon lots possible geometries of some alloys by designing a single special structure that best mimic the perfectly random real system. Following this idea, we have calculated the excited state properties of liquid water by ab-initio methods using a single, special, snapshot extracted among thousands resulting from a Molecular Dynamics run. We demonstrate that, once a special water configuration is chosen, its excited state properties will reproduce with sufficient accuracy the real system properties.

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## A unified description of ground and excited state properties of finite systems: the self-consistent $GW$ approach

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### Abstract

Due to their numerical cost,  $GW$  calculations are mostly performed perturbatively ( $G_0W_0$ ) following a density-functional theory (DFT) or Hartree-Fock (HF) calculation. At a higher computational cost, fully self-consistent  $GW$  (sc- $GW$ ) should ameliorate several shortcomings of the  $G_0W_0$  scheme, such as the violation of particle number conservation and the dependence on the starting point. So far, however, no clear verdict has been reached on the merits and shortcomings of sc- $GW$  in practical calculations, with preconceptions derived from isolated studies of model systems [1], precluding a systematic assessment. We have implemented a fully self-consistent  $GW$  scheme – based on the iterative solution of Dyson's equation – in the all-electron code FHI-aims [2]. sc- $GW$  total energies, calculated by means of the Galitskii-Migdal formula, agree well with full configuration interaction (CI) reference data and reduce the systematic overestimation of  $G_0W_0$  total energies based on DFT in the local-density approximation ( $G_0W_0@LDA$ ). The ionization energies, extracted from the spectral function of a set of 30 molecules, are in very good agreement with experiments, reducing the deviation of  $G_0W_0@LDA$  by 50%. For these molecules, we also observe that sc- $GW$  when initialized with different  $G_0$  always converges to the same  $G$  therefore removing the starting point dependence. The electron density at self-consistency is more localized in sc- $GW$  when compared to the LDA density, in line with the elimination of the self-interaction error. We conclude that sc- $GW$  provides a systematic improvement in the description of both ionization energies and total energies of finite systems with respect to conventional DFT-based  $G_0W_0$ . Furthermore, it provides a recipe to incorporate many-body effects in the ground-state electron density that are consistent with those in the excitation spectrum.

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# Simple preconditioning for time-dependent density-functional perturbation theory

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## Abstract

By far, the most common use of time-dependent density functional theory is in the linear-response regime, where it provides information about electronic excitations. Ideally, the linear-response equations should be solved by a method that avoids the use of the unoccupied Kohn-Sham states— such as the Sternheimer method— as this reduces the complexity and increases the precision of the calculation. However, the Sternheimer equation becomes ill-conditioned near and indefinite above the first resonant frequency, seriously hindering the use of efficient iterative solution methods. To overcome this serious limitation, and to improve the general convergence properties of the iterative techniques, we propose a simple preconditioning strategy. In our method, the Sternheimer equation is solved directly as a linear equation using an iterative Krylov subspace method, i.e., no self-consistent cycle is required. Furthermore, the preconditioner uses the information of just a few unoccupied states and requires simple and minimal modifications to existing implementations. In this way, convergence can be reached faster and in a considerably wider frequency range than the traditional approach.

# Unravelling the properties of graphene and nanotubes with Raman spectroscopy

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## Abstract

Recent results on the optical phonons and Raman spectra of graphene and nanotubes will be reviewed. Raman spectroscopy is shown to provide a powerful tool to differentiate between these two sp<sup>2</sup> carbon nanostructures which have many properties in common and others that differ. For example, in both graphene and nanotubes, the G and 2D Raman peaks change in shape, position and relative intensity with doping, grafting or pressure [1-5] but also with number of layers (respectively number of walls) [6]. These effects reflect the evolution of the electronic structure and electron-phonon interactions in such systems [7-9]. New results on opto-mechanical coupling in graphene will be discussed [10-12].

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# NMR and EPR with Density Functional Perturbation Theory

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## Abstract

Solid State NMR is sensitive to local structural and electronic material properties, which make it an important probe for material characterization with broad applications from material science and geology to biology and medicine. We recently extended GIPAW method, as implemented in Quantum ESPRESSO, to treat US and PAW pseudopotentials thus allowing us to address complex systems efficiently. Applications will be presented for the <sup>27</sup>Al NMR characterization of transitional alumina phases, including the catalytically important and poorly characterized  $\gamma$ -alumina phase, and for the assignment of Cholesterol <sup>13</sup>C NMR spectra to different crystalline polymorphs, which may help distinguish and assign spectra from gallbladder stones associated to different diseases and allow early diagnostic.

# The polarizability and hyperpolarizability of C and BN nanotubes. A quantum-mechanical simulation.

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## Abstract

The polarizability and hyperpolarizability of C and BN nanotubes. The polarizability, the first and second hyperpolarizability of BN and Carbon nanotubes of the (n,0) family have been evaluated by using a quantum-mechanical approach, a Gaussian basis set and the CRYSTAL code [1]. The Coupled Perturbed Hartree-Fock or Kohn-Sham Self Consistent perturbative schemes [2-3] have been implemented and applied to tubes of increasing radius (from (6,0) to (60,0)) [4,5]. The pure electronic and the ionic contributions have been evaluated, the latter through the FF-NR (finite field nuclear relaxation) scheme proposed by Bishop and Kirtman [6,7]. Longitudinal and transverse components of the three tensors are considered. Five different Hamiltonians (Hartree-Fock, LDA, PBE, PBE0 and B3LYP) are compared. The evolution with the tube radius is considered, and the trend towards the limit of infinite radius (that is, the hexagonal BN or the graphene monolayer) explored.

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## Auger Recombination and Impact Ionization from first-principles: from bulk to nanocrystals

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### Abstract

A detailed description, at the atomistic scale, of the dynamics of excess electrons and holes is fundamental in order to improve the performance of many optoelectronic devices. Among all recombination processes, non-radiative decay paths play a fundamental role in most of the semiconductor devices, such as optoelectronic devices and solar cells. In this work we show theoretical simulations of the Coulomb-driven Auger and Impact Ionization recombinations, which are the most important non-radiative recombination mechanisms in semiconductors, as proved both experimentally [1,2] and theoretically [3,4]. Understanding the physics behind these effects has crucial practical applications and represents an important step in the determination of the microscopic parameters that can affect solar cell and optoelectronic devices performances [5]. We present a first-principles study of the Auger Recombination for n- and p-type Si and GaAs bulk structures and of the Impact Ionization for Si nanocrystals of different size and doping. A complete ab-initio description of Auger Recombination processes combines DFT with many-body perturbation theory (in the GW approximation). We discuss the adopted method and present an accurate comparison between calculated and the experimental data pointing out the features that arise from the quantum confinement of the nanocrystalline form.

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# Excited state properties of $\text{TiO}_2$ surfaces and nanostructures

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## Abstract

We present results of a combined approach, TDDFT plus/vs MBPT, for the investigation of electronic and optical properties of  $\text{TiO}_2$  based systems. The interest for the material is mainly due to its application in catalysis, photocatalysis and hybrid photovoltaics. Therefore the analysis of optical absorption, excitonic behaviour and energy level alignment is a powerful tool to clarify the basic physical mechanisms underlying technological applications. We focus on description of nanocrystals and surfaces deriving from the anatase phase, also in presence of organic adsorbates, and discuss how to relate ab initio results to experimentally observed behaviour of the oxide.

## Optical characterization of Au nanowires on Si(111) surfaces

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### Abstract

An efficient route for fabricating regular and spatially-dense nanostructure arrays over a large area is to exploit self-organization of adsorbates on a substrate featuring a periodic pattern at the nanoscale. One such possibility is the engineering of one-dimensional (1D) quantum structures on stepped surfaces of silicon. Metal adsorbates act to stabilize flat and stepped (vicinal) Si(111) surfaces, leading to reconstructions having 1D features that are also interesting from a fundamental perspective. The exact structural and electronic properties of these monatomic wires depends on several factors, including the step width [1] and step morphology [2], the presence of adatoms [3], and spin-orbit coupling [3]. For instance, in the case of the prototypical Si(111)-(5x2)-Au surface reconstruction, adatoms appear to induce a spontaneous period doubling that is accompanied by an unusual "double" Peierls mechanism. A recent study [4] of 1-D indium chains on Si(111) demonstrated that low energy, anisotropic optical transitions probed by RAS are particularly sensitive probes of 1D behaviour, possibly because the largest 1D exotic effects are expected to be seen near the Fermi level. We present a joint experimental-theoretical study (carried out through an ETSF User Project) of the structural, electronic and optical properties of nominal and vicinal reconstructed Si(111)-Au surfaces, and interpret the measured reflectance anisotropy spectroscopy (RAS) data of these systems [5]. A phenomenological interpretation of the observed spectra has previously been proposed, but ab initio approaches are necessary for a thorough understanding of the structure and optical response. The role of adatoms, spin-orbit coupling, and higher order effects in the optical response will be addressed.

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## Phase transitions within the GW approximation

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### Abstract

The central concept of the single-band Hubbard model is the competition for the electrons between the tendency to localize for the on-site effective Coulomb repulsion  $U$  and the opposite tendency to hybridize and spread over other lattice sites, which gives rise to a finite bandwidth  $W$ . By varying the  $U/W$  ratio it is possible to obtain a transition from localized to itinerant electronic states. The realisation of this concept can be found in correlated electron materials, where by applying pressure it is possible to induce a transition from an antiferromagnetic insulating to a paramagnetic metallic phase. Here we will discuss metal-insulator transitions in prototypical real systems (e.g. MnO or NiS<sub>2</sub>) using the parameter-free GW approximation of many-body perturbation theory [1]. We will show that the GW approximation is a very useful tool to understand the effects of electronic correlations across the phase transition.

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## Momentum Distribution and Renormalization Factor in Sodium and the Electron Gas

S. Huotari, J. A. Soininen, T. Pylkkänen, K. Hämäläinen, A. Issolah, A. Titov, J. McMinis, J. Kim, K. Esler, D. M. Ceperley, M. Holzmann, and V. Olevano

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### Abstract

The homogeneous electron gas or jellium is one of the most fundamental models, canonical workbench to test different many-body theoretical approaches. Although really simple, still is very close to real solids, especially alkali metals, and sodium is one of its nature's closest realization. Here we present theoretical and also experimental results on the momentum distribution and the quasiparticle renormalization factor in sodium. From an x-ray Compton-profile measurement of the valence-electron momentum density, we derive its discontinuity at the Fermi wavevector. This yields for the first time an accurate measure of the renormalization factor, one of the most important quantities in many-body theory, that we compare with  $G_0W_0$  and quantum Monte Carlo calculations performed both on crystalline sodium and on the homogeneous electron gas. Our calculated results are in good agreement with the experiment. References: S. Huotari, J. A. Soininen, T. Pylkkänen, K. Hämäläinen, A. Issolah, A. Titov, J. McMinis, J. Kim, K. Esler, D. M. Ceperley, M. Holzmann, and V. Olevano, Phys. Rev. Lett. 105, 086403 (2010). A. Titov, V. Olevano, M. Ladisa, S. Huotari, K. Hämäläinen, and M. Holzmann, to be submitted.

## Current issues in the description of charged defects, the case of hydrogen in amorphous silica

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### Abstract

Defects in condensed matter are considered one of the most challenging issues in solid state physics. In particular, the computation of defect formation energies can be intricate while it is usually one of the first properties one aims to look at. We present results obtained with ABINIT [1] for hydrogen atoms in amorphous silica. Using a scheme [2] combining DFT and Many-Body Perturbation Theory in its GW approximation, we calculate the formation energies of different charged states of atomic hydrogen in amorphous silica. Contrary to previous applications of this method, the defect configurations are very different from one charged state to another. We explore different variations of the scheme to illustrate its limitations and present possible routes to overcome these.

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# Insights in the T-matrix approximation

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## Abstract

In many-body perturbation theory the self-energy  $\Sigma = iGW\Gamma$  plays the key role since it contains all the many body effects of the system. The exact self-energy is not known and approximations are needed. As first approximation one can set the vertex function  $\Gamma$  to unity which leads to the  $GW$  approximation, where  $G$  is the one-particle Green's function and  $W$  the dynamically screened Coulomb potential. Screening is important in the high-density regime and it is properly described within  $GW$ ; in the low-density regime, instead, other approximations are proposed, such as the T-matrix, which describes multiple scattering between two particles. In this work we give a rigorous derivation of the T-matrix approximation to the self-energy which puts it in a common framework with  $GW$ . This allows us to elucidate several aspects of this formulation, including the origin of, and link between, the electron-hole and the particle-particle T-matrix, the derivation of a screened T-matrix, and the conversion of the T-matrix into a vertex correction. The exactly solvable Hubbard molecule is used for illustration.

# TDDFT dynamics for strongly correlated model systems

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## Abstract

We discuss the nonequilibrium behavior of strongly correlated model systems (Hubbard model) via Time Dependent Density Functional Theory (TDDFT). Different approximations for the exchange correlation potential of TDDFT will be presented, and comparisons to exact and nonequilibrium Green's function solutions performed. Results from specific applications will be also shown, along with a mention to work in progress.

# Posters

(alphabetically ordered by last name of the first author)

## Coupling of excitons and defect states in boron-nitride nanostructures

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### Abstract

The signature of defects in the optical spectra of hexagonal boron nitride (BN) is investigated using many body perturbation theory. A single BN-sheet serves as a model for different layered BN- nanostructures and crystals. In the sheet we embed prototypical defects such as a substitutional impurity, isolated Boron and Nitrogen vacancies, and the di-vacancy. Transitions between the deep defect levels and extended states produce characteristic excitation bands that should be responsible for the emission band around 4 eV, observed in luminescence experiments. In addition, defect bound excitons occur that are consistently treated in our ab initio approach along with the "free" exciton. For defects in strong concentration, the co-existence of both bound and free excitons adds sub-structure to the main exciton peak and provides an explanation for the corresponding feature in cathodo and photo-luminescence spectra.

## A real-time approach to the optical properties of solids and nano-structures: the time-dependent Bethe-Salpeter equation

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### Abstract

Many-Body effects are known to play a crucial role in the electronic and optical properties of solids and nano-structures. Nevertheless the majority of theoretical and numerical approaches able to capture the influence of Coulomb correlations are restricted to the linear regime limit. In this work we introduce a novel approach based on a real-time solution of the electronic dynamics. The proposed approach reduces to the well-known Bethe-Salpeter equation in the linear-regime limit and at the same time allows to study correlation effects in nonlinear phenomena. We show the flexibility and numerical stability of the proposed approach by calculating the dielectric constants and the effect of a strong pulse excitation in bulk *h*-BN.

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## Ab-initio study of the Second Harmonic Generation process in the Si/CaF2 interface

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### Abstract

We present an ab-initio study of the linear and the non-linear optical properties of the Si/CaF2 interface. Second-Harmonic Generation (SHG) is a powerful selective spectroscopy technique for the characterization of surfaces and interfaces, and has been successfully applied to the measurement of the second-order dielectric susceptibility of the Si/CaF2 [1]. In our work, through the comparison between our ab-initio spectra and the experimental data, we investigate the importance of taking into account quasiparticle energies obtained with a scissor operator from the Kohn Sham structure, and the influence of the anisotropies present at the interface region, introducing the Local Field Effects in the Random Phase Approximation (RPA). We also analyse the effects of the silicon quantum confinement on the linear and non-linear response functions. All the calculations have been performed within the Time Dependent Density Functional Theory within the formalism of Ref. [2].

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# Unravelling the $\alpha - \gamma$ phase transition in Ce from the nanoscale to bulk

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## Abstract

The first-principles description of f-electron systems is currently regarded as one of the great challenges in condensed matter physics. The simultaneous presence of itinerant spd-states and localized partially occupied f-states and their mutual interaction in rare-earth materials gives rise to a rich variety of physical phenomena that continue to be a testing ground for electronic structure theories. Cerium, for example, undergoes an iso-structural  $\alpha - \gamma$  phase transition that is accompanied by a large volume collapse of 15% at room temperature and ambient pressure. In this work we apply the cluster extrapolation approach [1] that builds the cohesive energy of bulk Ce from corrections derived from clusters of increasing size. The electronic structure of each cluster is determined using hybrid density functionals (e.g. PBE0) and full exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA). In our calculations all electrons are treated on the same footing, unlike in dynamical mean-field theory (DMFT), that is frequently praised to be the method of choice for f-electron systems. For all clusters we find, at the PBE0 level, two stable configurations with different lattice constants and distinct electronic and magnetic properties, indicative of the phase transition in bulk Ce. Most surprising is that already the dimer exhibits a double minimum in the cohesive energy versus bond-length curve. Such a so-called ground-state bond-length isomer has never been observed experimentally before and might indicate that signatures of the phase transition in Ce are already present at the nanoscale. Experimental work inspired by our predictions is currently underway in the group of Prof. Wöste at the Free University in Berlin. While hybrid functionals incorrectly predict the high volume phase (linked to the  $\gamma$  phase) to be most stable at zero temperature, the correct energetic ordering is recovered in EX+cRPA where exact-exchange is screened in a physically meaningful way. This happens in correspondence with a higher density of states at the Fermi level for the  $\alpha$ -phase-like solution, in agreement with photoemission experiments [2]. Our zero-temperature EX+cRPA results complement previous LDA+DMFT studies (which for technical reasons are restricted to the high-temperature regime), and indicate that a first principles description of Ce within the framework of DFT is possible without invoking Kondo-like physics as in the case of LDA+DMFT.

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# GW and beyond approaches to quasiparticle properties in metals.

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## Abstract

We perform a comparative study of the performances of some standard approaches within the many-body perturbation theory. We calculate quasiparticle dispersion, lifetimes and spectral functions of aluminum and sodium. Calculations have been carried on in the *GW* approximation with a plasmon pole model (PPM), or with the contour deformation technique. We also accounted for vertex corrections either only in the screening (replacing the RPA dielectric function with the TDLDA or the Hubbard one), or both in the screening and in the self-energy (using the Del Sole *et al.* local vertex). Results show the failure of the PPM in describing the corrections far from the Fermi energy, as well as its impossibility in describing quasiparticle lifetimes and spectral functions. Calculations with a more refined screened interaction decrease the bandwidths and the lifetime of the quasiparticles compared with *GW* as well as induce tiny modifications in the spectral functions. The inclusion of the vertex also in the self-energy cancels the effects arising from the screening by pushing the results back toward the *GW* ones or even enlarging the differences.

## Ab initio study of the electronic properties of a-Si:H/cSi interfaces for photovoltaic applications.

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### Abstract

The use of heterojunctions between hydrogenated amorphous silicon (a-Si:H) and crystalline silicon (c-Si) has attract much attention in recent years for the fabrication of solar cells [1]. The passivation of the c-Si surface with a-Si:H films results in a great reduction of its surface state density, which allows the fabrication of high-efficient a-Si:H/c-Si heterojunction solar cells with efficiencies up to 23% [2]. Nevertheless, recent experiments have found that a-Si:H/c-Si heterojunction can suffer from light-induced degradation depending on the orientation of the c-Si substrate [3]. In order to shed some light into the origin of this negative effect, we have performed ab initio calculations of the electronic properties of a-Si:H/c-Si interfaces. For this purpose we have generated different heterojunctions using tight binding molecular dynamics. In the generated configurations, the crystalline part was oriented on the (100) direction - in both the 1x1 and 2x1 surface reconstructions - and on the (111) direction. The resulting atomic positions were used as the starting point of ab initio calculations. We will present and discuss preliminary results for the electronic properties and the density of states of the studied heterojunctions.

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## Plasmon dispersion in molecular solids: Picene and potassium-doped picene

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### Abstract

We investigate the dynamic response of pristine and potassium-doped picene, the first example of a new family of organic molecular superconductors, by combining first-principles calculations and state-of-the-art experimental tools. We find that charge-carrier plasmons in  $K_3$ picene have a negative or almost negligible dispersion, which deviates from the traditional picture of metals based on the homogeneous electron gas. We show how this finding is the result of the competition between metallicity and electronic localization on the molecular units. Conduction electrons alone give rise to the negative dispersion, which is reduced by molecular polarization and crystal local-field effects. This analysis allows us to obtain a general picture of the plasmon dispersion in metallic molecular crystals.

## First principles study of La on Au [111] surface : STM images and electronic structure properties.

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### Abstract

We study the electronic structure properties and the texture of lanthanum on (111) surface of gold imaged by scanning tunneling microscopy (STM) using the projected augmented-wave (PAW) approach to density functional theory. The local electronic density of states near the Fermi level and different regimes of tip-surface interactions as function of bias energies are explored. The bias energy and tip-surface distance turn out to be relevant for the contrast of the observed images. In order to analyze more quantitatively the orbital orientations and characters of bands on the surface we performed theoretical simulations of angle-resolved photoemission spectra (ARPES). The simulated spectra and STM images are compared with experiment.

## Stability of the sc phase of calcium

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### Abstract

As many materials, Calcium shows cristallorgaphic phase transitions under increased pressure. These transitions modify the physical properties of materials (giving rise, for example, to superconductiong proprieties). A sequence of phase transitions (fcc- $\rightarrow$  bcc - $\rightarrow$  sc - $\rightarrow$  Ca IV - $\rightarrow$  V) occurs in a wide range of pressure. Actually the sc phase of Calcium encounters some problems of stability. An ab-initio computation has been carried out to investigate if there exists a region in the Temperature-Pressure space in which the sc phase is stable. Two main contributions for the computation of the free energy have been considered: the electronic and phononic part. These contributions could be considered separately thanks to the adiabatic approximation. A detailed analysis has been done on the meshing of k-points, showing that the value of k-points needed to obtain a convergence of the energy ( $< 10^{-5}$  Ha) depends on the statistical distribution used (fermi dirac, cold smearing or gaussian). The ABINIT package has been used for these calculations.

Oganov A.R., Ma Y.M., Xu Y., Errea I., Bergara A., Lyakhov A.O. (2010). Exotic behavior and crystal structures of calcium under pressure. Proc. Natl. Acad. Sci.107, 7646-7651

# Many-body quantum simulations for organic systems: quasiparticle energies and electron-phonon coupling within the GW approximation

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## Abstract

On the basis of first-principles GW calculations [1,2], we study the quasiparticle properties of the guanine, adenine, cytosine, thymine, and uracil DNA and RNA nucleobases. Beyond standard  $G_0W_0$  calculations, starting from Kohn-Sham eigenstates obtained with (semi)local functionals, a simple self-consistency on the eigenvalues allows us to obtain vertical ionization energies and electron affinities within an average 0.11 and 0.18 eV error, respectively, as compared to state-of-the-art coupled-cluster and multi-configurational perturbative quantum chemistry approaches. Further, GW calculations predict the correct  $\pi$ -character of the highest occupied state, due to several level crossings between density functional and GW calculations. Our study is based on a recent Gaussian-basis implementation of GW calculations with explicit treatment of dynamical screening through contour deformation techniques.

Moreover, we study the electron-phonon coupling in the  $C_{60}$  fullerene within the mentioned GW approach [3], focusing on the lowest unoccupied t<sub>1u</sub> three-fold electronic state which is relevant for the superconducting transition in electron doped fullerenes. It is shown that the strength of the coupling is significantly enhanced as compared to standard density functional theory calculations with (semi)local functionals, with a 48% increase of the electron-phonon potential  $V_{ep}$ . The calculated GW value for the contribution from the Hg modes of 93 meV comes within 4% of the most recent experimental values. The present results call for a reinvestigation of previous density functional based calculations of electron-phonon coupling in covalent systems in general. [1] Xavier Blase, Claudio Attaccalite, Valerio Olevano, Phys. Rev. B 83, 115103 (2011).

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## Geometry and optical properties of nanostructured Si(110)

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### Abstract

The Si(110) surface is an important material for future technologies: on one hand its anisotropic nanostructured topology makes it a good template for growing nanowires (including Pb, Au and Sn nanowires); on the other hand it offers great potential for fabricating complementary metal-oxide semiconductor (CMOS) circuits with high hole mobility. The atomic structure is inherently complex: STM studies have suggested a 16x2 reconstruction consisting of equally spaced and alternately up and down stripes parallel to the [112] direction separated by atomic steps; along the stripes pair of pentamers have been observed. Up to now, however, no structural models have been proposed for the Si(110)-(16x2) reconstruction that explain in a consistent way the energetics, STM images and optical response data. The adatom-tetramer-interstitial (ATI) model proposed in [1] yields the lowest surface energy. We have studied ab-initio the optical properties and bandstructure of the ATI model, and compare our results to the experimental measurements: photoemission experiments [2] have identified the presence of four surface states. We also consider the new reconstruction model proposed in [3], in which the authors propose (based on precise STM imaging) a new model in which the pentamers are composed purely of adatoms, at difference with the ATI model.

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## Side-dependent electron escape in SiC-like graphene and graphane

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### Abstract

The structural and electronic properties of SiC-based two-dimensional (2D) crystals are studied by means of density functional theory and Many Body Perturbation Theory for the computation of electronic band structures. Both pure SiC sheets and their hydrides are studied. The structural and electronic properties cannot simply be interpolated between graphene and silicene. The replacement of C by Si atoms opens a large direct electronic gap and destroys the Dirac cones, and hydrogenation further opens this gap. Simultaneously, the electron affinity is significantly reduced for the escape of electrons, especially from the carbon-terminated side of the 2D SiC:H crystal, which shows a unique direction dependent ionization potential. This suggests the use of this material as electron-hole filter.

## Electronic and Transport Properties of Quasi-1D Wires of Biological Molecules

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### Abstract

Organic semiconductors are promising materials for low-cost and easy-to-process electronic and optoelectronic devices. Besides conjugated polymers, an important class of organic semiconductors are molecular crystals and/or stacks of high purity. Due to their high degree of structural order, such systems are ideal candidates for the investigation of the intrinsic excitations and charge-carrier transport phenomena in organic solids (1).

In the search for organic materials with good charge-transport properties, artificial stacks of biological molecules have been considered as attractive candidates in recent years (2,3,4). In this spirit, we present ab-initio DFT calculations of the structural, electronic, and quantum-transport properties (5) of quasi-1D wires based on guanine and eumelanin molecules (6). Hereby, a special focus is put on the results for the electronic bandwidths, effective electron and hole masses as well as the resulting consequences for potential applications.

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## Optical absorption spectra of brookite $\text{TiO}_2$

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### Abstract

The brookite phase of  $\text{TiO}_2$  has not been as extensively studied as anatase or rutile, due to difficulties in its experimental synthesis and the higher computation cost associated with its larger primitive cell. However, recent experiments have shown that brookite may enhance  $\text{TiO}_2$  photoreactivity, and this has boosted interest in better understanding the phase. Using density-functional theory and many-body perturbation theory techniques, we generate the optical spectra of brookite at several levels of approximation, with comparisons to anatase and rutile as well as experimental spectra. In particular, we examine the applicability of the effective energy technique (reducing the number of bands needed to converge a GW calculation) and the TDDFT long-range exchange-correlation kernel (in lieu of Bethe-Salpeter) as applied to  $\text{TiO}_2$ .

## Methanol molecules on a $\text{TiO}_2$ rutile (110) surface: basic properties leading to photocatalytic processes

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### Abstract

In this work we discuss the electronic level alignment and their respective charge properties of methanol molecules adsorbed on a  $\text{TiO}_2$  rutile (110) surface. Experiments show that photoexcitation can lead molecularly adsorbed methanols to dissociate on rutile (110) surfaces. Furthermore this system can lead to  $\text{H}_2$  production where methanol molecules act as hole acceptors speeding up the photocatalysis of the reaction. The underneath properties that lead the photocatalysis to take place have never been investigated and a comprehensive understanding is still lacking. We analyzed possible mechanism governing the process based on the results given by Density Functional Theory and many-body approaches to characterize the relative energy alignment of the states and electronic excitations, taking also into account the favorable geometric configurations of the complex and their energetic stabilities. Hole and electron sites involved in both the photodissociation and the photocatalysis will be discussed.

## Quantum detectors for spectroscopic instruments

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### Abstract

Optical spectroscopic methods are based on few characteristic essential phenomena of interaction of electromagnetic radiation with matter: a) absorption; b) fluorescence; c) phosphorescence; d) scattering; e) emission; f) chemiluminescence; One part of spectroscopic instruments block diagram is "radiation detector". Transducer that convert radiant energy into an electrical signal. There are two types of radiation transducers: one type responds to photons, the other to heat. Photon transducers are used largely for measurement of UV, visible and near-infrared radiation. In this paper a review is presented about properties and characteristic of these quantum detectors: sensitivity, spectral responsivity, photoresponse, signal-to-noise ratio.

Keywords: photon, quantum detector, radiant energy.

## Testing of the ABINIT implementation of the temperature dependence of the electronic structure

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### Abstract

The temperature dependence calculation based on the Allen-Heine-Cardona formalism and using a recently developed approach based on density functional perturbation theory (DFPT) has been implemented into ABINIT (Paul Boulanger's PhD thesis). This implementation does not take advantage of the symmetry of the crystal system and requires a large amount of memory. Also, more confidence in the implementation was expected through additional testing. This poster will present the improvements made to this implementation. First, the code was modified in order to decrease the memory requirement (by a factor fifty) while increasing slightly the computational time. Second, tests on primitive versus conventional cell were performed to see the effect of the use of symmetry operations. The possibility to calculate the Fan and diagonal Debye-Waller contribution for one q point has been added. A full convergence study up to a very dense q-point grid (2992 q-points in the irreducible Brillouin zone) has been done for Diamond. This gives us a converge value of about 420 meV (+- 10meV) for the zero-point motion correction. However this value is not in agreement with other existing calculation [1]. Extended testing are done to find the origin of this discrepancy.

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## Effects of confinement on water permeating through carbon nanotubes

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### Abstract

Nanochannels are of great interest in several areas: physics, chemistry, biology, optics, medicine, energy, and environment. They can be used for chemical sensing and molecule transport, proton transport, water pumping, or even nanofluidic manipulation. They make it possible to mimic cellular membrane processes. Their sizes allow for specific charge transport phenomena to occur, which is a key ingredient in the production of better fuel cells. They also can be used as very efficient water purifiers. The permeation mechanism has already been extensively studied, but there is still a lot to explore and understand regarding the changes in the properties of the water molecules themselves. Describing the permeation of water through nanochannels requires a multi-level modeling of the processes involved, since both the size of the system and the number of water molecules involved are often too large for a purely quantum-mechanical (QM) framework. With this in mind, we calculate how the confinement influences the electronic and optical properties of water molecules going through carbon nanotubes. We explore the role and importance of defects, as well as the changes induced by the presence of adsorbed molecules. We ultimately aim at determining whether an optical signature of confinement can be evidenced and evaluating which parameters are most influential on it.

## Potential Application of Si Polymorphs in Photovoltaics: Optical Absorption Spectra

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### Abstract

Si in the diamond structure, the naturally occurring Si polymorph under ambient conditions, constitutes one of the most intensively studied materials both experimentally and theoretically, since it is abundant in nature, can be grown in extremely good quality, and is of paramount technological importance as *the* key material in photovoltaics. However, its fundamental band gap at 1.2 eV is indirect and only phonon-assisted absorption processes with low probability can occur in the visible spectral range. The direct absorption edge at 3.2 eV lies in the ultraviolet spectral region which is unfavorable for the efficiency of photovoltaic applications due to the mismatch with the solar spectrum. Today a large variety of Si polymorphs is known, whereof some are semiconductors with direct gaps smaller than 3.2 eV. Here, we calculate the optical absorption spectra of the most promising candidates for strong absorption in the visible spectral range. We focus mainly on Si in the lonsdaleite structure, also known as wurtzite Si, which features a direct band gap of 1.6 eV matching ideally with the solar spectrum. Dielectric functions including excitonic and local-field effects are calculated by solving the Bethe-Salpeter equation. The optical absorption at the onset is compared to the absorption of diamond Si and discussed in terms of dipole allowed and forbidden transitions.

# Ab initio description of the Magneto Optical Kerr Effect

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## Abstract

The Magneto–Optical Kerr Effect,(MOKE) consists in the rotation of the light polarization plane incident on a magnetic material. Very recently the MOKE became the subject of intense experimental investigations mainly for two reasons. First it can be used to read magnetically stored informations by optical means in modern high density data storage [1]. Second, the MOKE is now regarded as a powerful probe in many fields of research such as microscopy for domain observation, surface magnetism, structural and magnetic anisotropies, etc... [2]. Despite the intense experimental research, very few calculations of the MOKE by first principles have been reported [3,4] and all within the independent particle approximations. Moreover it is common wisdom that the use of all electrons wave–functions is essential to get a correct description of the MOKE. In the present work we show that also pseudo–potential based calculations are quite accurate for metals like iron and cobalt. Moreover, for the first time to our knowledge, we address the inclusion of excitonic and local field effects in the description of the MOKE. In particular our target materials are transition–metal–doped dilute magnetic semi–conductors which are potential candidates for applications in the spintronic.

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## Search for efficient new materials for nonlinear optics

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### Abstract

A comprehensive understanding of the optical properties of solids is crucial for the improvement of non-linear materials and devices. It offers the opportunity to search for new materials with very specific properties. One particularly important process is second harmonic generation, where two photons are absorbed by the material and a photon, at twice the energy of the incoming photon, is emitted. Due to the success of approaches based on density functional theory to calculate the linear and the nonlinear responses of solids, we can now predict and simulate numerically the optical properties of complex materials. To develop high-power tunable laser sources, non-linear crystals (NLO) are commonly used, allowing the conversion of a fixed frequency to a shorter wavelength, through second order harmonic generation. The development of numerous NLO crystals led to significant advances in the laser device applications from ultraviolet to infrared spectral wavelengths and the synthesis of new materials has become an important issue. We will present the dielectric tensor and second-order susceptibilities for a large class of materials that can be used as efficient NLO crystals. In particular, we will study the role of the cristalloraphic structure in obtaining large values of the susceptibility.

## Influence of core electron polarization on electron energy-loss spectra

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### Abstract

In the calculation of electronic response spectra, the pseudopotential approximation is widely used. This is based on the assumption that the core electrons (which in this case include by definition all electrons not treated as valence electrons) and their polarization do not have any strong influence on the spectra. However, many experimental techniques measure spectra up to high energies, like for instance inelastic x-ray scattering experiments. In these cases, the absorption edges due to the (semi-) core states which are mostly included in the pseudopotential and not treated as valence electrons, appear as structures in the spectra. Due to the coupling via local-field effects and the connection of real and imaginary part of the dielectric function via the Kramers-Kronig relations, they can in principle influence the lower parts of the spectra as well. In the present work, we present a systematic study of these effects comparing energy-loss spectra computed for several materials within TDDFT. In particular, we compare calculations using different numbers of electrons, i.e., including or excluding the semi-core electrons from the spectra. Preliminary results, here presented, show small changes below the core edge which can be considered relevant if high accuracy is required. Moreover, we investigate the influence of local-field effects on the absorption edges and discuss the results by comparing to the case of silicon [1].

[1] H.-Ch Weissker et al., PRB 81 085104 (2010).

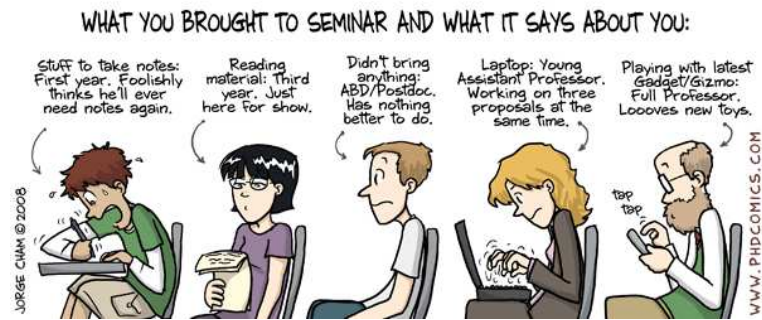
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# Notes







# Program

Tue 27	September
09:00	<b>Welcome</b>
09:30	J. Staehler
10:00	F. Rossi
10:30	A. Soudackov
11:00	<b>Coffee Break</b>
11:30	J. Fuks
12:00	N. Helbig
12:20	J. Ramsden
12:40	<b>Lunch</b>
14:30	X. Blase
15:00	F. Lépine
15:30	G. Mallocci
15:50	M. Rossi
16:20	E. Molteni
16:40	G. Gueorguiev
17:00	<b>Aperitif</b>
18:00	<b>ETSF meeting CT reports</b>

Wed 28	September
09:00	A. Gruneis
09:30	S. Bluegel
10:00	M. Guzzo
10:20	<b>Coffee Break</b>
10:50	L. Matthes
11:20	D. Kecik
11:40	F. Bechstedt
12:00	<b>Lunch+Poster</b>
14:20	G. Lani
14:50	L. Sponza
15:10	L. Stella
15:30	A. Stan
15:50	<b>Coffee Break</b>
16:20	J. Vinson
16:50	J. Kas
17:10	A. Marini
17:30	A. H. Larsen
18:00	F. A. Araujo

Thu 29	September
09:00	E. Tosatti
09:30	L. Venkataaraman
10:00	B. Oetzel
10:20	<b>Coffee Break</b>
10:50	M. Cazzaniga
11:20	N. Marom
11:40	M. Stankovski
12:10	<b>Lunch+Poster</b>
14:30	J. Neugebauer
15:00	N. Manini
15:20	B. XU
15:40	<b>Coffee Break</b>
16:10	S. Sharma
16:40	A. Mosca Conte
17:10	F. Caruso
17:30	L. Lehtovaara
20:00	<b>Social Dinner</b>

Fri 30	September
09:00	N. Bendiab
09:30	S. de Gironcoli
10:00	<b>Coffee Break</b>
10:30	R. Dovesi
11:00	M. Govoni
11:20	L. Chiodo
11:40	C. Hogan
12:00	<b>Lunch</b>
14:00	M. Gatti
14:20	V. Olevano
14:40	D. Waroquiers
15:00	<b>Coffee Break</b>
15:30	P. Romaniello
15:50	C. Verdozzi
16:20	<b>Closing remarks</b>
17:00	<b>CT meetings</b>