
YRM2009
B E R L I N

6th Nanoquanta-ETSF Young Researchers Meeting
REPORT

The Organizing Committee of the Sixth International Young Researchers Nanoquanta-ETSF Meeting (YRM2009) was composed of members of the ETSF-FUB Node located at the Theoretical Physics Department of the Free University Berlin. The full list of the organizing committee can be found on the conference web site: http://www.nanoquanta.de/yrm2009

This meeting was funded mainly through the "Deutsche Forschungsgemeinschaft" and the Ψ_k Network. The program included 8 hour-long Keynote talks and 29 short talks. There were 28 posters and a total of 89 participants, 35 of which were Bachelor and PhD students.

The YRM2009 brought together young researchers, comprising PhD students and postdocs working on applications and code development in diverse fields of theoretical physics. The scientific program covered areas from spectroscopy to electron correlation systems, molecular transport and nanostructural properties and some aspects of superconducting systems.

This meeting offered a unique opportunity for the attendees to have an open exchange of ideas and gain a better understanding of the theoretical and computational aspects of spectroscopy. Participants in their initial stage of research have the opportunity to discuss in more detail their project challenges, and the forum enables them to establish contact with other young researchers working in fields of mutual interest, as well as allowing them to build scientific relations with more experienced members of the community.

New developments in the study of the transport properties of molecular devices were presented, as well as some aspects of the transport properties of carbon nanotubes. The key concepts in the comprehension of the phenomenon of superconductivity were described, with particular emphasis on the recently developed superconducting DFT and its application to real materials.

State-of-the-art methods for treating electron correlations were covered. Recent advances in theoretical approaches to spectroscopic studies for diverse materials were exposed during the conference talks. The application of theoretical tools, including codes developed within the ETSF community, like ELK, Abinit, Octopus, DP, EXC, etc., to the study of nanostructures and biological systems provided an overview of the state-of-the-art tools available to aid in the understanding of electronic and spectroscopic properties of diverse molecular and solid state systems (i.e. dynamics of chemical and physical reactivity of molecular and biological systems, cubic ice and time-dependent studies of silicon).

The conference program also offered interaction with industrial and experimental participants, highlighting from one side the practical aspects of the gathered experiences in a theoretical research group during graduate studies and from another side the current collaborations between experimental and theoretical groups. Additionally, there was an opportunity for the participants to learn some aspects of gender and social issues that might hinder or facilitate research in different work environments.

We are pleased to report that the feedback from the participants was encouragingly positive.

BERLIN YRM 2009

Conference Program

	Tuesday 2	Wednesday 3	Thursday 4	Friday 5	Saturday 6
		Welcome			
09:00		Keynote 1	Keynote 3	C. Meisenbichler	
09:20		Transport	Spectroscopy	J. Wang	
09:40		Frank Ortmann	Eleonora Luppi	Keynote 5	
10:00		J. Hashemi	H. Huebener	Electron Correlations	
10:20		A. Lherbier	S. Sagmeister	Daniel Rohr	
10:40		Coffee break	Coffee break	Coffee break	
11:00		P. Myohanen	L. Espinosa Leal	P. Buczek	Departure
11:20		H. Ness	J. Vidal	F. Essenberger	
11:40		D. Nitsche	V. Garbuio	M. Guzzo	
12:00		Lunch break (12:00-13:30)	Lunch break (12:00-13:30)	Lunch break (12:00-13:30)	
13:40		Keynote 2	Keynote 4	A. Miglio	
14:00		Superconductivity	Nanostruc. & Bio	C. Panse	
14:20		Gianni Profeta	Daniele Varsano	G. Pegolotti	
14:40		E. Cannuccia	X. Declerck	R. Requist	
15:00		P. Cudazzo	K. Krieger	Coffee break	
15:20		Coffee break	Coffee break	Gender & social	
15:40		H. Glawe	A. Mosca Conte	issues talk	
16:00		M. Monni	N. Spallanzani	Kerstin Palm	
16:20	Arrival	Experimental talk	Industry talk	Closing remarks	
16:40		Karsten Heyne	Jan Werschnik		
17:00					
17:20		ETSF G. Bruant	Poster Session		
17:40		ETSF Software			
18:00	Welcome				
18:20	reception	Football			
18:40					
19:00				Social dinner	

Welcome to the Young Researchers' Meeting 2009! This is the sixth such conference for young electronic structure theoreticians and the second time that Berlin has hosted it.
Many of us are either beginning or partway though our PhDs or Postdocs, and as such, have an incomplete understanding of our research topic. The first purpose of this meeting is therefore to allow us to present and discuss our work as it stands without the inhibition that arises from being in the company of the leaders of our field. The second purpose is to establish new contacts and collaborations, some of which may remain throughout our careers, as well as gaining an overview of the ongoing research in our community. Lastly, of course, is to have fun: this is an exciting time to be at the forefront of computational physics, with new techniques and unprecedented computer power opening up previously unexplored areas.

We have been fortunate to obtain an outstanding venue for this year's meeting, in the newest hotel and conference center of one of Europe's most cosmopolitan cities. Berlin is vibrant day and night, with numerous cafes, museums, parks, clubs and bars, and we encourage all the attendees to make the most of their available free time over the next four days.

We would also like to express our gratitude to the people and entities who have made this conference possible, including Prof. E. K. U. Gross, Gabriele Hermann, Deutsche Forschungsgemeinschaft (DPG), The Psi-k Network, The European Theoretical Spectroscopy Facility (ETSF), and Freie Universität Berlin.

The YRM2009 Organizing Committee:

Ali Abedi, Tim Baldsiefen, Christophe Bersier, Alberto Castro, Kay Dewhurst, Florian Eich, Frank Essenberger, Andrea Floris, Henning Glawe, Elham Khosravi, Kevin Krieger, Andreas Linscheid, Danilo Nitsche, Stefano Pittalis, Antonio Sanna, Sangeeta Sharma and Angelica Zacarias

YRM 2009

Talks

Transport

Recent developments in theory of charge transport phenomena

Frank Ortmann *ortmann@ifto.physik.uni-jena.de*

ETSF Core Node Jena

Keynote Talk

The mobility is a concept that describes the current response of charge carriers to an applied electric field and is used to compare transport properties of different materials. High mobilities are required for electronics applications, and record values have been reported for graphene or, as an example for an organic semiconductor, rubrene. In order to theoretically derive this quantity along with its temperature dependence, different approaches have been used in the past which were based on the perturbative treatment of either the electronic coupling (bandwidth) or the electron-phonon coupling. The two limiting cases have been described within the narrow-band theory and the wide-band theory, respectively. In this talk I present a unified description which not only covers both limits but also the intermediate regime. Particular emphasis is put on the transition between band conduction and hopping motion. The novel approach is discussed in application to the organic crystal naphthalene.

Electronic and Transport calculation of Carbon NanoBuds

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Having high carrier mobility as well as stable structures, nanotubes stood up as one of the main candidates for micro and nanosize electronic devices. Capability of adopting different transport properties according to their geometry make them more favorable and yet subtle to work with. For these, nanotubes and in particular carbon nanotubes have been explored and studied both experimentally and theoretically in great details. Defects, impurities and imperfections, as an inevitable but not always unfavorable characterization of a real-world nanotube, have also attracted many attention. These are important since they can modify the electronic properties of nanotubes to some extend. Albeit not as muchas nanotubes and graphene, other carbon-based structures waere an active area of research as well. Recently a combined carbon nanostructure has been discovered. Carbon NanoBud, CNB, as it is called in the original work, is a buckyball covalently bonded to a single-walled carbon nanotube, SWCNT, and it is expected to open a space for more innovative application of nanotubes in micro and nanoelectronics. In order to employ them, we need careful studies of their properties both in theory and experiment. In this work, we are trying to investigate electronic structure and transport properties of CNBs. We will show that the transmission function is highly sensitive to any change in the neck region (the region where c60 is attached to the nanotube).

Charge Transport Simulation, an ab initio and tight-binding coupled approach.

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ETSF Core Node Louvain-la-Neuve

We present a Kubo-Greenwood transport formalism in real space which allows to investigate all transport regimes, including localization phenomena. Transport calculation are performed within the tight-binding framework but with disorder potential coming from ab initio calculations. As an example we will present results on charge transport in chemically doped 2D graphene.

A many-body approach to quantum transport dynamics: Initial correlations and memory effects

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ETSF Associate Node Jyväskylä

We study time-dependent quantum transport through a correlated quantum dot model system by means of time propagation of the nonequilibrium many-body Green's function. The theory is an extension of the Kadanoff-Baym approach for finite inhomogeneous systems to open inhomogeneous systems and generalizes the steady-state Meir-Wingreen approach to transient time-domain including the initial correlations and memory effects. We find that the electron correlation effects have a large impact on transient and steady state currents.

Many-body Effects and Inelastic Electronic Transport through Nanoscale Devices

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ETSF Core Node York

We study the effects of the interaction between electrons and atomic vibrations in the context of electronic transport through molecular nano-devices. We use a technique based on non-equilibrium Green's functions and different approximations for the corresponding electron self-energies. We apply this technique to model systems describing a lead-molecule-lead heterojunction and calculate both the current and current-current correlation functions. We discuss the effects of the e-ph interaction and of the potential drop on the current and on the inelastic electron tunneling spectra. We suggest the possibility of obtaining a molecular-scale nano-switch. We also briefly discuss the fluctuation-dissipation theorem in the context of non-equilibrium transport.

Time-dependent electronic transport in two and three dimensions

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ETSF Core Node Berlin FU

We present a recently suggested scheme for the description of time-dependent transport with the focus on two- and three-dimensional systems. The implementation of this algorithm into the time-dependent density functional theory framework requires the propagation of the Kohn-Sham orbitals of an infinite system starting from its ground state. For the calculation of the continuum orbitals of this extended system we propose an effective Lippmann-Schwinger equation. The time-evolution is carried out by a modified Crank-Nicholson propagation scheme. This time-dependent scheme naturally allows time-dependent phenomena like transient effects, time-dependent potentials and AC biases but also recovers the steady-state limit for DC-biased systems.

Electron-Phonon interaction and Superconductivity

Electron-phonon coupling,superconductivity and related phenomena

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CNISM, University of L'Aquila Physics Department

Keynote Talk

Superconductivity is one of the most spectacular manifestations of quantum mechanics.
Since its discovery, the theoretical prediction of the superconducting critical temperature represents a challenge for solid state physics.
In this talk, We introduce some fundamental concepts in the theories of electron-phonon superconductivity.
Starting with the original formulation of the BCS, we, then, introduce the theoretical framework at the base of the Migdal-Eliashberg theory, to end with the formulation of the SuperConducting Density Functional Theory (SCDFT).
We review the recent successes of SCDFT on real materials and discuss possible new applications on recent discovered superconductors.

Exciton-vibron interaction in one dimensional conjugated polymers

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ETSF Core Node Rome

The giant one dimensional excitonic localization, combined with the peculiar electronic character, dictate the exited state properties of conjugated polymers (CP). These one dimensional systems are attracting an increasing interest because of their potential application as opto-electronic devices [1]. The prediction of solitons in polyacetylene (PA), in 1979 [4] by the Nobel Prize J.R. Schrieffer, is maybe, the most stricking evidence of the strong interaction between electronic and atomic degrees of freedom in CP. Similarly, optical absorption experiments, often carried out at room temperature, reveal interesting features in the spectra, that are not described within the state-of-the-art theoretical tools. The axial polarizability spectrum is dominated by bound excitons characterized by an asymmetric line-shape, and appearing together with strong vibronic-induced side bands [2,3]. In contrast, the ab-initio description based on the solution of the Bethe-Salpeter (BS) equation [5], is clearly inadequate. As showed in the case of solids [6], the standard BS equation is insensitive to the temperature, as it is usually solved in the frozen atoms approximation, neglecting the coupling with molecular vibrations. In this talk I will present an ab-initio approach to the exciton-vibron interaction. I will discuss how to describe, in an accurate manner, the role played by vibrations and temperature in the axial polarizability of CP.

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[3] K. Pichler et al., J. Phys.: Condens. Matter **5**, 7155 (1993)
[4] W. P. Su, J. R. Schrieffer, A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979) [5] M. Rohlfing and S. Louie, Phys. Rev. Lett. 82, 1959 (1999)
[6] A. Marini, Phys. Rev. Lett. 101, 106405 (2008)

Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen

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ETSF Core Node San Sebastian

We present a first-principles study of the electron-phonon interaction and the prediction of the superconducting critical temperature in molecular metallic hydrogen. Our study is able to single out the features which drive the system towards superconductivity: mainly, a rich and complex Fermi surface and strongly coupled phonon modes driving the intra- or intermolecular charge transfer. We demonstrate that in this simple system, a very high superconducting critical temperature can be reached via electron-phonon and Coulomb electron-electron interactions.

Doped $CaCuO_2$: a Superconducting DFT study

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In the past, density-functional theory for superconductors (SCDFT) has been applied to a wide range of systems ranging from weak-coupling (Mo, Al, Ta) and strong-coupling (Nb, Pb) simple metals to highly anisotropic systems like MgB_2 and CaC_6 with great success — the calculated T_c, superconducting gaps and specific heat are in good agreement with experiment. One of the motivations leading to the development of the framework of Superconducting DFT was the discovery of the *cuprate high-temperature superconductors*. However, it is not clear in how far the present approximations neglect phenomena important only in this class of materials. Exploring where we stand in this respect, calculations have been performed on a structurally simple high-temperature superconductor, namely the doped, non-magnetic *infinite-layer* material $CaCuO_2$. DFT-calculations have been performed for the normal state using the PBE GGA approximation for the exchange-correlation functional. The full phonon dispersion and the electron-phonon coupling matrix elements have been calculated. Finally, SCDFT calculations were performed taking a Thomas-Fermi screened Coulomb interaction into account when solving the fully anisotropic self-consistent gap equation. In this talk, the results of these calculations will be presented, alongside perspectives for future improvements in our approximations.

Multiband superconductivity in sulfur under high pressure: a first principles study.

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SLACS (Sardinian Laboratory for Computational Materials Science) CNR-INFM

We present a first-principles study of the electron-phonon interaction and superconducting critical temperature in body-centered orthorhombic (bco) sulfur under high pressure (up to 200 GPa), using the density functional theory applied to the superconducting state. We study the behavior of superconducting properties across the bco to phase transition, experimentally corresponding to the appearance of a charge-density wave and to a depression of the Tc value. Remarkably, we find that the origin of this discontinuity can be physically ascribed, to a large extent, to the evolution of the multiband character of superconductivity in this compound.

External Talks

Experimental and theoretical ties: do's and don'ts

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Unraveling reaction mechanisms on the molecular level is one of the most interesting and challenging topics in physics, chemistry and biology. However, most reactions relevant in everyday life concern molecules of hundreds to several thousands of atoms that are difficult to characterize with experimental or theoretical methods. One way to tackle that problem is to use simplified models reflecting only the essential parts of the investigated reaction mechanism. The crucial point in using this strategy is the reliability of the separation of essential and dispensable parts. This requires precise knowledge of fundamental parameters, such as 3D structure, wave functions in the ground and excited state, energy of transitions, orientation of transition dipole moments, and couplings.
We combine experimental approaches with high level calculations to achieve more accurate results on fundamental reaction mechanism parameters. With our approach we are able to identify the character of the lowest electronic transitions in molecules (e.g. anthracene derivatives [1], see figure). Furthermore, we improved polarization resolved femtosecond spectroscopy to determine the 3D orientation of selected electronic transition dipole moments in Chlorophyll a [2] and the laser dye Coumarin 314. In general structural information on configurations can be deduced from the combined approach resulting in a refinement of the used models.

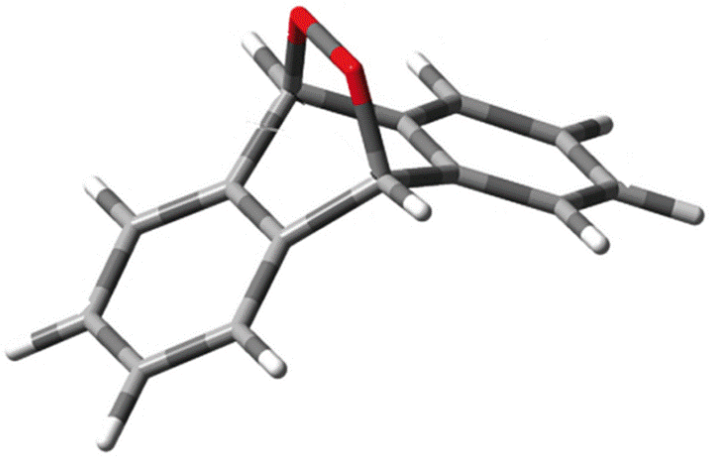

Figure: 3D structure of anthracene-9,10-endoperoxide in its electronic ground state. The endoperoxide bridge can be dissociated or cleaved upon excitation.

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The ETSF at the time of its fourth call for proposals

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European Theoretical Spectroscopy Facility

The European Theoretical Spectroscopy Facility [1] is carrying out its fourth call for proposals. How does it work? What are the results? A first contract with an industrial user is being signed. What does it look like? /Nanoquanta/ is over; a project called "ETSF-I3" has replaced it. What is the difference? In this talk, I will try to give some answers to the questions above.

[1] www.etsf.eu

Spectroscopy

Non-linear spectroscopy and related phenomena

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Keynote Talk

Non-linear electromagnetic phenomena in the optical region mainly occur with high intensity laser beam as a sufficient intense radiation is needed to modify the optical properties of a material system. In fact, the beginning of the field of the non-linear optics is often taken to be the experimental evidence of the second-harmonic generation by Franken et al. [1] in 1961, shortly after the demonstration of the first working laser in 1960[2]. In the second-harmonic generation experiment by Franken et al. [1], a ruby laser beam at 6942 $\mathring{A}$ was propagated through a quartz crystal and an ultraviolet radiation from the crystal at 3471 $\mathring{A}$ was observed. This was the first non-linear optical effect were a coherent input generates a coherent output. Since 1961 numerous non-linear optical phenomena have been discovered, creating revolutionary changes in optics technology. In condensed matter the theoretical description of non-linear process become particularly difficult because the non-linear response of the medium has to be coupled with the induced fields. A panoramic on different optical phenomena will be given, together with a detailed theoretical derivation of the susceptibility beyond the linear response.

[1] P. A. Franken and *et al.*, Phys. Rev. Lett. **7**, 118 (1961)
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Towards Second Harmonic Generation in Bulk Silicon

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Second Harmonic generation is dipole forbidden in centrosymmetric media, like cubic Si. Therefore one has to consider quadrupole responses in order to describe bulk contributions to non-linear surface spectroscopy experiments of such media. A perturbative expansion of the transition matrix elements for the second-order susceptibilty is unfeasible so that a different approach is needed. Furthermore, when describing optical response, TDDFT is not strictly valid for finite **q**-vectors of the light field. We propose to employ time-dependent-*current*-density-functional theory to overcome these limitations. To this end, several conceptual questions regarding transverse response and current-DFT have to be understood already in the linear case.

Time-dependent density functional theory versus Bethe-Salpeter equation: An all-electron study

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We perform first-principles calculations for the macroscopic dielectric function within an all-electron full-potential framework, i.e., the linearized augmented planewave (LAPW) method. To this extent we pursue two different routes, which are, on the one hand, many-body perturbation theory (MBPT) by solving the Bethe-Salpeter equation (BSE), and time-dependent density functional theory (TDDFT), on the other hand. The implementation into one program package, i.e., the EXC!TiNG code, allows a direct comparison of these approaches, in terms of accuracy as well as efficiency. We briefly review the theory, and describe in detail the quantities being specific to the LAPW method. We show results for simple systems as well as for organic semiconductors.

Towards a gauge invariant method for molecular chiroptical properties in TDDFT

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We present an efficient scheme to calculate the chiroptical response of molecular systems within time dependent functional theory using either a real-time propagation or a frequency-dependent Sternheimer method. The scheme avoids the commonly used sum over empty orbitals and has a very favorable scaling with system size. Moreover, the method is general and can be easily implemented. In the present work we implemented it using a real-space pseudo-potential representation of the wave-functions and Hamiltonian. The specific use of non-local pseudo-potentials implies that a gauge correction term in the angular momentum operator must be included, to ensure that the total scheme is fully gauge invariant. Applications to small organic chiral molecules are shown and discussed, addressing some deficiencies of present exchange-correlation functionals to describe the absolute position of the excitations. However, the shape or sign of the dichroism spectra comes out in excellent agreement with available experiments.

Paradox of CuIn(S,Se)2 bandgap: a GW study.

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During the past year, Cu(In,Ga)(S,Se)2 (CIGS) thin-film solar cell have emerged as a technology that can challenge the current hegemony of silicon solar cell. This is due to the extraordinary optical and structural properties of CIGS. Among all their properties, the most remarkable one is their insensitiveness to any structural or stoichiometric deviation. We used scCOHSEX+G0W0 methods to investigate the dependence of bandgap on some structural parameters. We found a huge dependence of the bandgap on the anion displacement contradicting most of the experiments. We explained this discrepancy by a coupled process between defect formation and structural relaxation.

Proton disorder in the optical properties of cubic ice

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Ordinary ice has a hexagonal crystal structure (ice Ih). A metastable cubic crystalline variant of ice exists, where oxygen atoms are arranged in a diamond structure (ice Ic), and the hydrogen ones are disordered, still obeying the Pauling ice rules. It is produced at temperatures between 130-150 K, and is stable for up to 200 K, when it transforms into ice Ih. The proton disorder in ice has a role in several properties such as growth condition and thermic properties [1,2] and many works about phase transitions from proton disordered to proton ordered ices can be found in literature. Moreover, depending on the proton ordering, some ice phases can also present ferroelectric or antiferroelectric behaviours [3,4]. In recent years, the excited state properties of hexagonal ice have been studied within many-body perturbation theory (MBPT) [5]. The electronic and optical properties of cubic ice, instead, have never been calculated accurately: only tight-binding [6,7] and density functional theory (DFT) [8,9] calculations have appeared in the literature. Moreover, in several of these studies the proton disorder is not taken into consideration. Here, we present MBPT calculations of the optical spectrum of cubic ice exploiting model cells with different level of proton disorder, including the ferroelectric phase. We also compare our results for the excited states properties with ice Ih and with liquid water.

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[7] L. Resca et al., phys. stat. sol. b **81**, 129 (1977)
[8] W. Y. Ching et al., Phys. Rev. Lett. **71**, 2840 (1993)
[9] W. Y. Ching et al., Ferroelectrics **153**, 25 (1994)

Biomolecules, Nanostructures and Quantum Dots

Bio-molecules, nano-structures and quantum dots: What they are and how to study them.

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ETSF Associate Node Modena and
ETSF associate member of San Sebastian Node

Keynote Talk

In the last decades nano-structures have attracted the attention of a huge part of the scientific community. An introduction to the technological potentiality of these systems will be provided, focusing on their electronic and optical properties related to the reduced dimensionality.
State of the art of the ab-initio computational frameworks used for the study of such systems will be reviewed and particular attention will be devoted on bio-systems and their possible use in molecular electronics.

First principle study of the electronic properties of boron nitride nanoribbons

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ETSF Core Node Louvain-la-Neuve

Non-passivated zigzag-edge boron nitride nanoribbons exhibit a metallic behaviour and some spin polarization effects comparable to what one observes in graphene nanoribbons. These effects can be explained through the existence of particular localized states. A first characterization of electronic transport properties will also be presented.

Calculation of ultra-short laser pulses for selective bond breaking

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Within the last years femtosecond physics has become a very ambitious field in research. Due to sophisticated techniques in experimental physics, laser pulse shaping of ultra-short pulses is fully feasible today. With such pulses physical processes in the femtosecond regime can be controlled. One example for these processes are chemical reactions, which can be controlled by selective bond breaking of the reactants. Here, we present some first calculations based on time-dependent density functional theory and quantum optimal control theory, which show how the laser pulses that induce the selective bond breaking can be theoretically predicted.

A theoretical study of the first steps of the mechanism of vision by GW and BSE

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The mechanism of vision is present in most of the living beings. In superior animals, this mechanism is supported by a complex apparatus, but the ability to transform external optical solicitations in chemical signals is also present in the most primitive forms of life such as bacteria. In all the cases, the first and most important phase of the mechanism is the photo-isomerization of the rhodopsin retinal, that is a change of the retinal structural geometry induced by the absorption of a photon. Despite the importance of this process and several experimental and theoretical studies on this topic, the photo-isomerization is not fully understood yet. The reasons rely on the difficulty of several theoretical methods (many of whom are based on TDDFT) to provide an accurate description of the optical properties of the retinal along all the phases of the process. In this work we study the retinal's photo-isomerization by GW and BSE methods obtaining results in good agreement with the experiments. We give a substantial contribution to the comprehension of the still obscure aspects of the vision process, and investigate the reasons of the failure of most of the methods and approximations commonly used in TDDFT in providing a qualitative description of it.

Photo-excitation of a light-harvesting supra-molecular triad: a Time-Dependent DFT study

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We present the first time-dependent density-functional theory (TDDFT) calculation on a light harvesting triad carotenoid-diaryl-porphyrin-C60. Besides the numerical challenge that the ab initio study of the electronic structure of such a large system presents, we show that TDDFT is able to provide an accurate description of the excited state properties of the system. In particular we calculate the photo-absorption spectrum of the supra-molecular assembly, and we provide an interpretation of the photo-excitation mechanism in terms of the properties of the component moieties. The spectrum is in good agreement with experimental data, and provides useful insight on the photo-induced charge transfer mechanism which characterizes the system.

External Talks

From Abbe to Zernike: Experiences of a physicist in the optics industry

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Jena-optics

The talk will start with the career of Ernst Abbe, who can be considered as a role model of an industrial physicist. His scientific work will lead us from optics theory to the profession of an optical designer. We will leave Abbe at this point and meet Frits Zernike who leads us along the optics parade from a designer's point of view. Finally and briefly, I will show where electronic structure calculations enter the story. Along the talk I would like to tell you about my experiences as a physicist (and ex-young researcher) in the optics industry.

Special Topics

Xml Technology in the EXCITING DFT Package

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ETSF Associate Node Leoben

The presentation illustrates on hand of the exciting DFT package the capabilities of XML as file format standard, for both, input and output processing. This includes: assisted input, simulation monitoring, data visualization, and quality assurance. It should become clear, that it is not only new technology but also allows new approaches to simulation setup, simulation archives, and data analysis.

Relaxation models of the (111) zinc-blende IV-IV semiconductor surfaces: a first-principles calculation

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Northwestern Polytechnical University, Xi'an China

The relaxations of the (111) zinc-blende IV-IV semiconductor surfaces are studied using density function theory (DFT) calculations. In a systematic study, the general relaxation trends of different surfaces are explained using atomic Pauling electronegativity and the calculation results of spin density distributions.

Electron Correlation

Electron Correlation Functionals

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Institute of Physics, Technical University of Lodz, Poland

Keynote Talk

In the first part the definition for electron correlation is given for three different theories. The Hartree-Fock (HF) method as a first approximation to the Schrödinger equation is reviewed. The HF reference gives rise to the traditional definition of electron correlation. Contributions to electron correlation are analyzed. It is pointed out that the kinetic energy, the electron-nuclear interaction energy as well as the electron-electron interaction energy contribute. The exchange and correlation holes are discussed.
The concepts of Density Functional Theory (DFT) are reviewed including the Hohenberg-Kohn and Kohn-Sham theorems. It is shown that electron correlation in DFT only contains contributions from the kinetic energy and the electron-electron interaction energy. Jacob's ladder of approximations to the exchange-correlation functional in DFT is presented. Difficulties in development of the most sophisticated functionals are highlighted.
Finally, Density-Matrix Functional Theory (DMFT) is presented. Electron correlation in DMFT only contains contributions from the electron-electron interaction. A recent breakthrough in DMFT functional development is presented.
In the second part Time-dependent DFT (TD DFT) is presented. It is shown how linear response properties can be calculated from TD DFT. A few approximations in TD DFT are presented.
[1] A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry*
[2] C. Fiolhais, F. Nogueira and M. Marques (Eds.), *A Primer in Density Functional Theory*
[3] D. Mazziotti (Ed.), *Reduced-Density-Matrix Mechanics*
[4]M. Marques, C. Ullrich, F. Nogueira, A. Rubio, K. Burke and E. K. U. Gross (Eds.), *Time-Dependent Functional Theory*

Energies and life times of magnons in Heusler alloys

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Heusler alloys are promissing materials for spintronic applications, particularly when they feature half-metallic ground state. We have studied energies and life times of spin-waves in several Heusler systems using linear response density functional theory. We show that the number of magnon modes can be smaller that the number of magnetic atoms in the primitice cell of the crystal. Neither the latter effect, nor the Landau damping of magnons can be described in the standard Heisenberg model. Furthermore, it is shown that the half-metallicity of the system results in long-living acoustic spin-wave excitations whereas the optical modes are strongly damped by Stoner spin-flip excitations. The Stoner continuum leads not only to the damping of spin-waves but also to a renormalization of their energies.

Comparative study of LSDA and LSDA+U scheme: an application to transition metal oxides

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Transition metal oxides (TMO) are prime examples of the failure of the local spin density approximation (LSDA) within density functional theory (DFT). Strong correlations beyond the LSDA have been identified as the main cause of this failure. The simplest procedure for including these effects within single particle DFT calculations is the so called LSDA+U method. In order to highlight the differences between LSDA and LSDA+U method in this work, we perform a careful analysis of NiO, CoO, MnO and FeO, and determine the gap, moment, band-structure, density of states, and electron localization function (ELF) as a function of the parameters U and J, as well as the underlying exchange-correlation functional. These differences will lead to better insight required not only for understanding the physics of strong correlations but also for developing improved functionals within DFT capable of treating strongly correlated systems.

Exchange and correlation effects in the electronic properties of transition metal oxides: the example of NiO

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The purpose of my work is to investigate the role of exchange and correlation effects on the electronic structure of nickel oxide (NiO), in particular on the nature of the insulating energy-gap, by means of ab-initio methods. As a prototype of strongly-correlated materials, the electronic structure of NiO has been extensively studied, experimentally and theoretically [1,2,3,4]. However, the origin of its gap is still under debate. Direct and inverse photoemission experiments are the most direct experimental way to measure the band structure of solids. From a theoretical point of view, we have to describe changes in the number of particles of the system. Many-Body Perturbation Theory (MBPT) — where the key quantity is the one-particle Green's function, i.e. the propagator of an electron/hole — is the appropriate tool to describe and understand photoemission. The GW approximation from MBPT [5] includes dynamical screening and correlation effects beyond H-F. The standard GW approach calculates first-order corrections of the LDA eigenvalues, but is not reliable on NiO since the Kohn-Sham band structure is too poor to be used as a starting point. It is thus necessary to go beyond standard GW. I used the COHSEX approximation [5,6], a static approximation of GW, to achieve self-consistency in energies and wavefunctions, to obtain a better starting point for the GW step. The GW+COHSEX photoemission spectrum gives an energy-gap of about 5 eV, in good agreement with experiment. In particular, I obtain similar results as another more time-consuming approach beyond perturbative GW [4]. In GW the screening is due to classical noninteracting charges. An improvement to GW would consider the screening between quantum interacting particle instead. An attempt to follow this way in the $GW\Gamma$ approximation [7] has shown no improvement in the spectrum.

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[6] Bruneval, F., Vast, N., and Reining, L., Phys. Rev. B **74** 045102 (2006)
[7] Del Sole, R., Reining, L., and Godby, R. W., Phys. Rev. B **49** 8024 (1994)

Transparent Conducting Oxides (TCO): a case study

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TCOs are a class of oxides with increasing importance in many technological applications like solar cells and flat panel displays. They are optically transparent, wide gap semiconductors or insulators which also display good electrical conductivity, due to doping or intrinsic defects. Among the TCOs most widely used, we have focused on tin oxides (SnO_2 and the less stable SnO) as a case study. In order to explore their electronic bulk properties, we first performed DFT ground state ab-initio calculations within a PAW implementation,employing both LDA and GGA exchange-correlation functionals. The Sn semi-core d states, relevant especially in SnO_2, are explicitly taken into account as valence states in the PAW atomic data sets. To improve the description of the band gap,we have subsequently applied one-shot GW corrections.

Magnetic properties of transition metal doped Si nanocrystals

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In order to investigate the magnetic and spin-related properties of nanoparticles we examine transition metal doped semiconductors. In particular Si nanocrystals (NCs) doped with Mn and Fe atoms are under investigation. We consider two different impurity positions (substitutional and interstitial) and two different exchange and correlation (XC) functionals (GGA and GGA+U). To verify Hund's rule for the NC systems we have analysed the spin and charge distribution in these systems in detail. A strong dependence of the total magnetic moment on the energetic position of the metal d-states and hence, on the used XC functional could be observed.

Visualizing charge fluctuations in graphite

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Starting from ab initio calculations performed with ABINIT and DP, it has been possible to calculate the induced charge density that a generic system shows in response to an external perturbation. Working in the framework of TDDFT, we have calculated the linear response of a graphite system in the random phase approximation. Our work has been devoted to show the charge fluctuations for different external perturbations and to discuss their relation with plasmons. Our method also allows to investigate their physical nature, for example by discovering which electrons partecipate to oscillations.

Adiabatic and nonadiabatic dynamics via the one-electron reduced density matrix

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The dynamics of an electron system driven by a time dependent external potential $v(r,t)$ will be adiabatic if $E_{gap}\tau/\hbar \gg 1$, where E_{gap} is the minimum instantaneous energy gap (between the first excited state and the ground state) and τ is the characteristic time scale for $v(r,t)$. We introduce an adiabatic functional approximation for the Bogoliubov-Born-Green-Kirkwood-Yvon equation of motion for the one-electron reduced density matrix (one-matrix). The only necessary input for the approximation is a "reconstruction" of the ground state two-matrix in terms of the one-matrix, which is available from many of the existing ground state energy functionals. Tests for a simple model system find that the approximation performs quite well, even beyond the adiabatic regime naively expected on the basis of the above adiabaticity condition. Nonadiabatic transitions and substantial admixture of excited states become evident for lower values of τ. The adiabatic one-matrix functional approximation is compared with the adiabatic extension density functional approximation, and it is found that both are able to describe some of the nonadiabatic effects but that their performance depends sensitively on the strength of the electron-electron interaction. A correction that improves the description of nonadiabatic effects is proposed.

External Talks

Gender & science

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Visiting Professor at University of Graz, Department of Molecular Biology

This talk gives a short overview about the main three research fields in the Gender & Science Studies with a focus on the Gender & Physics debate. After a description about the asymmetric priviledge distribution concerning the gender specific positioning and status assignment (staff organisation level) I will continue with the content level which deals with the analysis of the genderspecific character of physical theories. The last part will treat the genderspecific structure of physical epistemology, i.e. the double character of a specific concept of objectivity as neutral and at the same time symbolic masculine, the "gods trick" (speaking from a non responsible position of a socially nowhere about everything) and some other topics regarding the structural level of scientific thinking. This three levels, the staff, the content and the structure of scientific research, cannot be separated from each other and must be considered together, as I will explain in the last part of the talk.

YRM 2009

Posters

X-ray diffraction, crystal structure and spectral features of the optical susceptibilities of single crystals of ternary borate oxide lead bismuth tetraoxide $PbBiBO_4$

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The all electron full potential linearized augmented plane wave method has been used for an ab initio theoretical study of the band structure, the spectral features of the optical susceptibilities, density of states, and electron charge density for PbBiBO4. Our calculations show that the valence band maximum (VBM) and conduction band minimum (CBM) are located at centre of the Brillouin zone resulting in a direct energy gap of about 3.2 eV. We have synthesized the PbBiBO4 crystal by employing a conventional solid-state reaction method. The theoretical calculations in this work are based on the structure built from our measured atomic parameters. We should emphasize that the observed experimental X-ray diffraction (XRD) pattern is in good agreement with the theoretical one, confirming that our structural model is correct. Our calculated bond lengths show excellent agreement with the experimental data. This agreement is attributed to our use of the full potential calculations. The spectral features of the optical susceptibilities show a small positive uniaxial anisotropy.

Optoelectronic properties of intermediate-band photovoltaic materials from first-principles calculations

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Thin-film photovoltaic materials represent one of the most currently developed technologies in the quest of more efficient, lower-cost solar cells. The compounds we present here are derived from the chalcopyrite semiconductor CuGaS−2 and the spinel MgIn−2S−4. In

this compounds, some of the group-III atoms are substituted by transition metals to give rise to the intermediate-band material. The electronic structure is thus modified in a way that an isolated partially filled narrow band appears between the valence band and the conduction band of the host semiconductor. This particular electronic structure allows these materials to absorb low energy photons, creating electron-hole pairs not only by the promotion of an electron directly from the valence band to the conduction band (like in conventional semiconductors), but also due to the absorption of two low-energy photons that can promote an electron from the valence band to the intermediate band (IB) and another one from the IB to the conduction band. This implies a more efficient use of the solar spectrum that could increase the efficiency of the cell up to 63.2 % much higher that the theoretical limit of conventional cells (40.7%).
Due to the lack of experimental results of these materials, it is necessary for the proper understanding of the intermediate band formation, to study their properties theoretically in order to predict their suitability for high efficiency photovoltaic purposes. Our aim is to describe and predict by ab- initio methods their properties and especially the contribution of the new intermediate band to their optical properties. For that purpose we need a precise description of the electronic structure of the systems and since this precision is not reached with standard DFT methods, the use of other advanced ab-initio methods is necessary. We have performed GW calculations for some of the intermediate-band materials and we present some exact exchange (EXX) and DFT+U results for comparison.
Optical spectra within the RPA approximation, and within the Time Dependent DFT approach, have also been studied.

Quantum Dynamics with time-dependent density matrix.

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The time-dependent density matrix formalism or BBKGY offers a natural way to do quantum dynamics, but as to the hierarchy structure of it, truncation of these equations at some level and introducing an appropriate approximation is an inevitable step towards applications. By keeping the first two equations which include up to three-body reduced density matrix (3RDM) we can capture almost all interesting physics of the system, provided

substituting 3RDM with a good approximation in terms of 1RDM and 2RDM. In this work we replace 3RDM with a Hatree-Fock like approximation, investigating consequences of it.

GW without empty states: Beyond the COHSEX approximation

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The GW approximation (GWA) to the self-energy[1] has proved to be very successful in the calculation of quasi-particle energies for a wide range of solids. However, the GWA is computationally expensive which is mainly due to the slow convergence with the number of unoccupied states that have to be taken into account. This has led to to search for simplified approximations such as the COHSEX approximation[1] in which there is no sum over unoccupied states. However, the COHSEX quasi-particle energies are, in general, not close to the GW energies. A different strategy is to look for a more efficient approach to calculate the GW self-energy such that only a small number of unoccupied states are required[2]. In this way the GW accuracy is retained. In this work we will go beyond the COHSEX approximation and obtain an approximation to the GWA without empty states but with a better accuracy than the COHSEX approximation.
[1] L. Hedin, Phys. Rev. **139**, A796 (1965)
[2] F. Bruneval and X. Gonze, Phys. Rev. B **78**, 085125 (2008)

Correlation effects in photoemission spectra of transition metals: 3BS theory faces experiment

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3BS [1,2] is a non perturbative, many-body method to compute spectral functions of solids.

It takes into account correlation effects due to strong local Coulomb interaction (described via the Hubbard model), thus allowing to correct the single-particle density of states or band structure of the system and to study its quasi-particles properties. Here we use 3BS to study photoemission spectra of iron, cobalt and nickel, in a detailed comparison with, on one hand, DMFT results [3] and, on the other, recent experiments of angle- and spin-resolved photoemission spectroscopy [4]. In addition, 3BS has been embodied into a one-step model simulation of photoemission, with the inclusion of matrix elements as well as surface effects [5].
The aim of our work is to establish a comparison between different theoretical methods and to determine to which extent the features we see in the experimental spectra of these transition metals are ascribable to correlation effects.
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[2] F. Manghi et al., Phys. Rev. B **56**, 7149 (1997)
[3] I. Di Marco et al., unpublished
[4] J. Sanchez-Barriga et al., unpublished
[5] J. Minar et al., unpublished

A paradigmatic metal with semicore and spin polarization effects: bulk iron

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We present the calculation of electronic and optical properties of bulk iron using ab initio methods. Iron poses several interesting theoretical challenges: it is a metal with highly correlated 3d electrons and it shows band magnetism. In the present work intraband transitions are described using an original method based on a Taylor expansion of the dispersion relations across the Fermi energy. The comparison of calculated dielectric function at the RPA level with available experimental data shows some discrepancy due to the presence of the 3d electrons, not well described within DFT. On the contrary, optical conductivity and loss function are in good agreement with experiments and the inclusion of semicore levels in the pseudopotential allows the description of the edge. We also discuss the origin of the structures present in the EEL in the low and medium energy region of the

spectrum.

Theoretical spectroscopies of near-free-electron metals

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We address simple elemental metals, mainly bulk aluminum and sodium, by ab-initio methods. We start from optical properties including intraband transitions using an original method. We than move on to the calculation of the loss function both for zero and finite momentum transfer taking into account electronic correlations beyond RPA. Finally we address photoemission spectroscopy with quasiparticle properties, using standard GW with contour deformation, which allow us to investigate band structure corrections, quasiparticle lifetimes and the spectral functions

Spin polarized circular dichroim in resonant photoemission from ferromagnets

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A first ab-initio description for resonant photoemission is given within the LMTO and real space multiple scattering approach. Resonant photoemission, together with resonant inelastic X-ray scattering, is a widely used technique in X-ray spectroscopy to study electronic correlations, local and non local magnetic properties, geometry-related properties. It is essentially the process through which a photon is absorbed, the electron is excited in the conduction state, and the system relaxes by emitting another electron (it is also called resonant Auger partecipator channel). We discuss here the first results on spin polarized

circular dichroism from a Fe surface.

Non-equilibrium inelastic electronic transport: beyond the self-consistent Born approximation for electron-phonon interactions

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We consider the problem of the interaction between particles (electrons e and phonons ph) in the context of electronic transport in nanoscale devices. We use the so-called Keldysh Green's functions technique and consider the non-equilibrium steady state regime. The many-body effects are included in the form of self-energies treated within a self-consistent conserving approach. Different levels of approximation are used for the corresponding e-ph self-energy. We consider the lowest order diagram in the e-ph coupling (i.e. the so-called self-consistent Born approximation SCBA) and second order diagrams (i.e. so-called double exchange diagram or lowest order GW-like diagram). Results for the equilibrium and non-equilibrium spectral functions as well as for the current are presented for a wide range of parameters. We show that it is necessary to go beyond the commonly-used SCBA to obtain correct results for all the range of e-ph coupling.

CVV Auger spectra for broad band systems with hole-hole interaction

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I shall report on our work in progress towards the inclusion of the hole-hole interaction, together with a proper description of transition matrix elements, in a single ab initio framework for the description of core-valence-valence (CVV) Auger spectra. More commonly, the hole-hole interaction in the final state is either neglected (which is a reasonable starting

approximation for broad band systems), or a band average is taken as an approximation for the transition matrix element (affecting the lineshape especially for broad bands). Hence, we aim at introducing the hole-hole interaction in our implementation of the CVV Auger spectrum calculation. The method is based on a Kohn-Sham calculation for the emitting atom embedded in a host with cylindrical symmetry (e.g., simple metal, simple metal surface). Transition matrix elements are evaluated consistently on the same basis function as the one-particle Green's function. The non interacting two particle Green's function is then evaluated and provides the final-state density of states. We are then looking forward implementing a Dyson-like equation due to Cini and Sawatzky for the two particle Green's function with hole-hole interaction, which is exact when the valence shell is closed. The bare Coulomb interaction can be computed on the same footing as the matrix elements, while further development is necessary to consider the screening.

A simple ab-initio calculation of the optical gain in Si-nc

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Optical gain in Silicon nanocrystals (Si-nc) has been demonstrated in a large variety of experimental conditions. In several papers, the origin of the optical gain was ascribed to the active role of radiactive interface states formed at the interfaces between the Si-nc and the embedding Silicon oxide. The analysis of the optical-physical-chemistry properties of the materials will support the understanding of the correlation between the Si-nc/dielectric system properties and the experimental conditions. Understanding and controlling the properties of these new materials at the nanoscale is becoming a crucial step. In this contest, theory plays a fundamental role, allowing one to describe the electronic excitations of complex systems with efficient and accurate ab-initio methods. In this presentation, results obtained in the study of the optical and electronic properties of simple Si-nc will be discussed. Again, a detailed analysis of the radiative and non-radiative (Auger) decay processes, that play a crucial role in the description of the optical gain dynamic under pump pulse, will be given. This represents a first preliminary step of a project that will be finalized to the resolution of a set of channel specific rate equations.

Spatial Resolution in Electron Energy-Loss Spectroscopy

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First, we have studied the spatial distribution of excitations (plasmons) in Carbon systems using ab initio calculations within the framework of time-dependent density functional theory (TDDFT). Second, we present an approach to study spatially resolved EELS in the low loss region (less than 40 eV), explicitly taking into account for non-local effects of the dielectric function.

Clusters and Nanowires of anatase TiO_2: structural, electronic and optical properties as functions of the nanomorphology

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Titanium dioxide (TiO_2) nanostructures are nowday widely investigated for their multipor-pose capabilities in several fields of social and commercial relevance. The primary task is the design of optimized nanodecives for application in the solar energy conversion or the photocatalytic water splitting[1]. We show here the dependece of the structural, electronic, and optical properties of TiO_2 nanowires (NW) and clusters (NC) from their morphology and surface coverage, by means of density functional theory (DFT) calculations. Based on the synthesis features of real nanosamples[2], we defined an anatase TiO_2 NC by modifying a bipyramidal morphology and then used this NC as a chain repetition unit in the NW. We studied the effect of the size confinement by considering different diameters of the NWs. We then analyzed the influence of the surface coverage by adsorption of simple water-derived species, given the importance of the surface termination in determining the TiO_2 photoactivity. By varing the direction of elongation and the lateral surfaces of the NWs we investigated the influence of the morphology on the overall properties of these

TiO_2 nanostructures. At last we show the variation of the optical properties of anatase TiO_2 in going from the extended crystal to the nanostructured forms, within the random phase approximation, time-dependent DFT and many-body corrections schemes.
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[2] J. Polleux, N. Pinna, M. Antonietti and M. Niederberger, Adv. Mater. **16**, 436 (2004).

In strong correlation we trust? The paradimg of the V2O3 case

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Aim of our work is to study through an ab initio theoretical approach the paramagnetic insulting phase of V_2O_3 compound, in order to understand better the metal-insulator phase transition subdues by V_2O_3. It has been shown that at DFT level it's not possible to describe properly the insulating paramagnetic phase because of a poor treatment of the strong electronic correlation for such systems with d- or f- incomplete shell. Moreover the comparison of DFT density of state with the experimental one is not possible until including many body effect such the ones arising from a direct photoemission spectroscopy. Within a traditional ab initio density functional scheme, the Kohn-Sham eigenvalues can' t be used for an appropriate description of the electronic bands structures, leading in particulaer for such a system (VO_2, V_2O_3) to an underestimation or even to a closure of the photoemission band gaps. Moreover, from the experimental point of view it has been shown that adding small amount of Cr into the V_2O_3 a sharp metal-insulator transition arises as a function of both Cr concentration and pression at room temperature. Since to the best of our knowledge all the theoretical calculation present in the literature concern only V_2O_3 without really taking into account the Cr dopant atom, we decide to perform ab initio calculation by considering Cr-doped V_2O_3 supercell system in order to point out which role the presence of the dopant plays on the electronic structure during the metal-insulator paramagnetic transition of the V_2O_3. For what concerne the optical properties, we will show absorption and eels spectra have been calculated to investigate through an abinitio approach the low-lying dd excitations and their differences in the metallic and insulating phase of the V_2O_3.

An alternative route to the self-energy.

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Calculations of quasi-particle band structures in solids rely more and more on the many-body technique known as the *GW approximation*. While in general very successful, it is known to fail for a few systems. The GW method consists of introducing (and then approximating) a quantity –the *self-energy* Σ– in the equation of motion (EOM) (known as Dyson equation) of the one particle Green's function **G**. This strategy allows to include in a handy quantity all the many-body effects beyond the Hartree-Fock approximation and, most importantly, to recast the equation in a closed form, allowing for an iterative calculation of **G**. Here we propose an alternative route: in place of Σ we work the exact EOM, which involves the functional derivative of G respect to a perturbing external potential, and direclty solve the resulting set of first order non-linear differential equations. To validate this approach we apply it to a two-site Hubbard hamiltonian, for which an exact solution is available; this will be an essential and enlightning step to ultimately apply it to real systems.

Liouville-Lanczos Approach for Molecular Excited States

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An algorithm based on a mathematical framework optimized for large-scale and extensible linearized time dependent density functional theory calculations is presented. First, the density response of linearized TDDFPT is cast into two subspaces particularly suitable for oblique projection algorithms, and then using non-Hermitian Lanczos algorithm corresponding time dependent equations are solved. The biggest advantage of this approach is that once the corresponding reduced form of the Liouvillian is calculated, observables like the absorption spectrum within all the viable range of applicability can be obtained almost

instantaneously. The source of the presented algorithm is available under GNU license and can be found as a part of quantum-espresso project at http://www.qe-forge.org .

Optical Response of Small Cationic Xenon Clusters from TDDFT

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Upon ionization, rare-gas (like Ar and Xe) clusters shift their absorption spectrum from the ultra-violet to the visible. This happens as bonding becomes much stronger due to the removal of an electron from a strongly antibonding orbital. We have studied the absorption spectrum of small cationic xenon clusters (Xe+n, with n=3,...,35) by means of TDDFT. These calculations include relativistic effects through the use of relativistic j-dependent pseudopotentials in a 2-spinor formulation of the Kohn-Sham equations.

Exploring the Pr-Pfr transition of biliverdin

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Biliverdin is the phytochrome found in bacteria, and has been recently observed as a crystal in its Pr form within the surrounding protein. Its Pr-Pfr transition has been studied both experimentally and theoretically. The most involved region of the molecule around the chromophore has been identified, though no definitive answer has been given for the final geometry. The protonation state of the Pfr form is not clear either, and the mechanisms of the possible proton transfers occuring are still unknown. Adding to the confusion, recent studies suggest that the transition might involve a rotation around a single bond in addition to isomerisation. Due to steric clashes, the rotation would in turn cause further

conformational changes in the protein environment. Until now this process has been eluded because of its complexity. I will present our latest achievements in looking for the transition path.

Towards experimental spectra calculations using linear-scaling density functional theory

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I will present preliminary work towards the calculation of excited states within the linear-scaling density functional code ONETEP, which will eventually lead to the capability of determining experimental spectra.

Exploring the random phase approximation: application to the CO adsorption puzzle, bulk metals, and weakly bonded molecules

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Density-functional theory within the generalized gradient approximation has been immensely successful in describing the ground state properties of a diverse range of materials. However, inherent strong self-interaction effects and the absence of van der Waals interactions are two prominent examples of GGA's failures. The random phase approximation (RPA) as formulated within the adiabatic connection fluctuation dissipation theorem presents a promising way to overcome these dificiencies. However, despite the considerable interest the RPA has generated, a comprehensive assessment of its performance is not available. Using CO@Cu(111), a selection of bulk metals, and the benzene dimer–a prototypical π-conjugated system as examples, we demonstrate the performance of

the RPA for different types of systems. We show that the potential-energy surface of CO adsorbed on Cu(111) can be correctly described within RPA at a quantitative level. The binding energy of the benzene dimer, on the other hand, is considerably underestimated.

Ab initio study of CO2/Ni(110)

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The peculiarity of the interaction of CO2 with Ni(110) with respect to other metallic surfaces has been recently pointed out by combined theoretical and experimental studies. A deeper investigation including the analysis of the electron localization function and simulations of scanning tunneling microscopy images is presented here. The role of steps, of under coordinated surface sites and other defects are also exploited. Preliminar results for adsorption on a NiCu alloy are also discussed, in order to gain information about the possibly different behaviour of the Ni and Cu metals with respect to the CO2 interaction.

Hubbard model: GW vs exact solution

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The Hubbard model [1] is widely used to deal with the physics of strongly-correlated materials. In particular, the two-site Hubbard molecule is a good test system because it can be solved exactly. Therefore, it can be used to study the physics of excitations and to see how the GW approximation to the self-energy performs, where the main problem is, and how one might go beyond. Here we use the two-site Hubbard model with one electron, in order to understand the self-screening problem that the GWA suffers from [2,3].
[1] J. Hubbard, Proc. Roy. Soc. A **276**, 238 (1963)

[2] W. Nelson, P. Bokes, P. Rinke, R. W. Godby, Phys. Rev. A **75**, 032505, (2007)
[3] P. Romaniello, D. Sangalli, J. A. Berger, F. Sottile, L. G. Molinari, L. Reining, and G. Onida, J. Chem. Phys. **130**, 044108 (2009)

Ac-AlanLysH+ in vacuo: secondary structure of polyalanine peptides

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Predicting the structure and stability of peptides is a challenge, and in vacuo studies provide unique, well-defined conditions to match state of-the-art experiments and theory. We here present a combined force field (OPLS) / density-functional theory (DFT) study of the polyalanine peptides Ac-AlanLysH+ (n=5,10,15), for which earlier experiments indicate helical secondary structure [1]; the results are verified by comparing to room-temperature multiphoton IR vibrational spectra measured using the FELIX free-electron laser (part I). For Ac-Ala5LysH+, we pre-screen O(105) candidate structures in the force field, and then use DFT in the generalized gradient approximation with van der Waals corrections (GGA+vdW) in the FHI-aims code [2] to refine a wide range of low-energy conformers. We show (i) how the LysH+ termination acts to stabilize helical structures, (ii) a close energetic competition between different helical motifs (, 310) in the Ala5 part. Both GGA+vdW and the vibrational spectra are consistent with an -helical motif. We address systematic frequency shifts between theoretical (harmonic) and the measured spectra, and the role of anharmonicities through extensive ab initio molecular dynamics simulations.
[1] R. Hudgins, et al., JACS **120**, 12974 (1998)
[2] V. Blum, et al., Comput. Phys. Comm., accepted (2008)

Ab-initio calculations of MnO in different crystal structures and magnetic orderings

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Antiferromagnetic transition-metal oxides (TMOs) are materials of great interest for applications in new magnetic materials (e.g. dilute magnetic semiconductors) and spintronics. There have been a couple of - theoretical as well as experimental - studies on the ground-state properties of MnO, but only few including also crystal structures different from the experimental rock-salt structure. We present an ab-initio study of structural, electronic, and magnetic properties of MnO using density-functional theory (DFT). The results obtained within the (semi)local generalized-gradient approximation (GGA) are compared with findings taking into account an additional on-site interaction U (GGA+U) and results using the non-local hybrid exchange-correlation functional HSE03. Besides the rock-salt structure, which is the natural ground-state structure of MnO, we focus especially on the properties of MnO crystallizing in wurtzite structure, which is the ground-state structure of e.g. ZnO, a potential host material for dilute magnetic semiconductors. For each crystal structure we consider six different magnetic orderings and compare them with experimental and, as far as available, other theoretical data. In particular we present our findings that GGA, GGA+U, but also HSE03 show shortcomings in the description of ground-state properties of MnO and that a treatment of exchange and correlation beyond the (semi)local one is necessary for a more accurate description.

PAWs for thought: PAW+GW on Transparent Conducting Oxides

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We present a case study of the PAW method applied to the electronic structure of ZnO, a transparent conducting oxide with many important applications. The significant overlap

of Zn 3d-orbitals with 3s and 3p semi-core states necessitates the inclusion of these in ground-state- and GW calculations, as we show with a comparative study. Furthermore, we have tested two approaches to the calculation of overlaps between plane-wave basis functions and the PAW spherical augmentation functions, and have found the use of the exact expression of Arnaud & Alouani (PRB **62**, 4464) crucial for GW calculations on these systems. In contrast, the use of the approximate expression of Shishkin & Kresse (PRB **74** 035101) leads to an incorrect ordering of GW bands. Finally, we present preliminary results of Quasiparticle Self-Consistent GW applied to ZnO wihtin the PAW approach.

Levels of self-consistency in the GW approximation

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We investigate the effect of self-consistency in the GW approximation, on several observables. We propose a new GW scheme which yields results in very close agreement with fully self-consistent GW calculations, at a computational cost comparable with the G0W0 scheme. The proposed method can be easily implemented for solid state systems for which fully self-consistent GW calculations are difficult to perform.

Electron correlation and spin-orbit coupling in alloys and alloy surfaces: Au_2Gd

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The electronic structure of gold-gadolinium alloys is investigated using DFT and LDA+U, and including the spin-orbit interaction. Fine details of magnetism and correlation influence the band structure of monolayer-thick alloys, which are compared to ARPES experimental

data.

Temperature effects on the electronic and optical properties of silicon clusters

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The simulation of nanostructures has been a topic of great interest over the last years. In particular the *ab initio* calculation of the optical and electronic properties, i.e., of those properties which are important for the construction of solar cells and opto-electronic devices, has developed rapidly.
However, these *ab initio* calculations are numerically very demanding. They have been limited to relatively small systems and to zero temperature. Full molecular dynamics in order to study temperature effects due to lattice vibrations are restricted to a small number of atoms.
The combination of semi-empirical methods for the determination of geometries and of lattice vibrations in nanocrystals is a promising way to overcome these limitations. In these calculations, the structure is treated using classical or semi-empirical molecular dynamics, after which the electronic and optical properties are calculated *ab initio*.
In the present work we treat temperature effects on the optical spectra and on the electronic structure of silicon-hydrogen clusters as they occur in industrial PECVD plasma reactors. The geometry including temperature-dependent lattice vibrations is treated using model-potential molecular-dynamics simulation [1], while *ab initio* calculations in density-functional theory are presented using the adiabatic local-density approximation (ALDA, also knows as TDLDA) and, for comparison, independent-particle results.

[1] N. Ning, G. Dolgonos, W. Morscheidt, A. Michau, K. Hassouni and H. Vach, Computational Methods in Science and Engineering, **1**, (2007)

YRM 2009

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PSI-K WORKSHOP FINANCE REPORT

Title of the Workshop	6th Nanoquanta-ETSF Young Researchers Meeting
Workshop Organisers	Ali Abedi, Tim Baldsiefen, Christophe Bersier, Alberto Castro, Kay Dewhurst, Florian Eich, Frank Essenberger, Andrea Floris, Henning Glawe, Elham Khosravi, Kevin Krieger, Andreas Linscheid, Danilo Nitsche, Stefano Pittalis, Antonio Sanna, Sangeeta Sharma and Angelica Zacarias
Location of the Workshop	Berlin, Germany
Dates of the Workshop	June 2nd-6th, 2009
Total Grant from Psi-k	4,200

EXPENDITURE

(Please complete the tables using numbers ONLY in the amounts fields - the spreadsheet will calculate the totals for you)

WORKSHOP DELEGATES / SPEAKERS			
Name and Country of Claimant	**Travel**	**Conference Fee**	**Total (€'s)**
Christian Panse	€ 60.00	€ 300.00	€ 360.00
Adreas Schroen	€ 76.00	€ 300.00	€ 376.00
Nicola Spallanzani	€ 77.90	€ 300.00	€ 377.90
Javad Hashemi	€ 253.00	€ 300.00	€ 553.00
Ali Hussain Reshak Al-Ja'Ary	€ 68.00	€ 300.00	€ 368.00
Laura Ratcliff	€ 130.60	€ 300.00	€ 430.60
Christian Mechenbichler		€ 300.00	€ 300.00
Johanna Fuks		€ 300.00	€ 300.00
Leonardo-Andres Espinosa		€ 300.00	€ 300.00
Ali Akbari		€ 300.00	€ 300.00
Giulia Pegolotti		€ 300.00	€ 300.00
Marco Govoni		€ 300.00	€ 300.00
		Total Travel & Accommodation	**€ 4,265.50**

WORKSHOP REFRESHMENTS / CONFERENCE DINNERS			
Date	**Tea / Coffee**	**Lunch / Dinner**	**Total (€'s)**
			€ -
			€ -
			€ -
			€ -
			€ -
		Total Refreshments	**€ -**

MISCELLANEOUS EXPENDITURE	
Details	**Total (€'s)**
Total Miscellaneous	**€ -**

Total Travel & Accommodation	**€ 4,265.50**
Total Refreshments	**€ -**
Total Miscellaneous	**€ -**
TOTAL EXPENDITURE	**€ 4,265.50**