

# 8th ETSF Young Researchers' Meeting



ANTONIO SANSEVERI  
SOCI TURRI MADRI  
PAULI SANSEVERI  
PRINCIPIS FELIX  
SOCIETATE INGENIO  
SARINO FORTUNA ADMIRAE  
QUI OPUM UOXORE  
IN ADULESCENTIA AMISSA  
CALIDIS DIEB  
SUVENIENS COMPTATIBUS  
SATE SUINO PARLISSET  
PROPTEREAQUE  
MTRIA PROXIA TURPHAM OMNES  
PISACRASSIT  
EDINO COGNITE  
TANDEN EDICORIBUS  
BECOX SACRERDIO  
HURDQ-TIMPLO ARBAS  
SAPICITATE MORUM DIGNOS  
MO-ED-NEPT-AN- MDCCCLVII  
AT-DIA LEXIS OMNIBUS DICUNT  
NON DATUM ESSE  
HUMANI IMMACLITATE  
UT MAGNA SINE VITI VIRTUTES  
CAUSTANT  
RAYMENTIS SANSEVERI  
PRINCIPIS FELIX  
NE QSD PATRI NE QSD VIRITATI  
EDIFICARET  
EDINGER EDIGUM  
SUCCESSIONEM POMPHEIUM  
CIRLIT

16 - 20 May 2011  
Naples, Italy

## Welcome all of you!!

who came traveling far in search of wisdom (...and maybe good pizza (?)).

We are very happy to welcome you to the 8th ETSF Young Researchers' Meeting taking place in beautiful Naples. We hope, you are looking forward as much as we do to the 4 and a half days ahead of us, stuffed with lots of interesting talks, posters and exciting and fruitful discussions.

Regarding the scientific organization, we mostly stuck with last years concepts. Every day will start with a by-now-almost-traditional keynote talk, where the speaker (deemed by the young researchers' community to have a deep knowledge of their subject and having gracefully agreed on playing teacher for one day), in addition to talking about his/her own work, will introduce the general concepts of the working field. Thanks a lot for their work and dedication. In addition, we replaced the usual non-scientific talk by a scientific one, Lorenzo Stella will give an introduction to Quantum Monte Carlo, which most of us have heard but few know much about. Thanks to him, too.

Everyday will have one or two discussion sessions, we hope you will use them intensively. To trigger even more discussions, we asked you to hand in questions beforehand, which are also supposed to be addressed. The other thing we asked was a short work description your working fields. This information can be found at the end of this booklet. We hope, it will be useful to find and get into contact with exactly the right person, who you might need to discuss with.

The official poster session is Tuesday evening, although the posters can stay up until Friday.

In addition to the (organized) scientific part we hope, we left enough free space for you to enjoy the company of your colleagues and the nice people and city around you.

Finally we would like to thank the University of Naples for hosting us and last but not least you all for your time and effort. We hope, you will find it worth it.

Yours sincerely, the organizers,

Michele Amato, Fulvio Berardi, Ivo Borriello, Roberto D'Amico, Leonardo Andrés Espinosa Leal, Johanna Fuks, Nicole Helbig, Amilcare Iacomino, Yann Pouillon, Lorenzo Stella, Jessica Walkenhorst, Marius Wanko

## About

The European Theoretical Spectroscopy Facility (ETSF) is a network carrying out state-of-the-art research on theoretical and computational methods for studying electronic and optical properties of materials. The ETSF gathers the experience and the know-how of more than 200 researchers, including professors, postdocs and Ph.D. students, in Europe and the United States, facilitating collaborations and rapid transfer of knowledge. Moreover, the ETSF is a user facility dedicated towards providing support and services for ongoing research in academic, government and industrial laboratories. The main objective of ETSF is to broaden access to the knowledge and the expertise in the field of theoretical spectroscopy across the public and private sector.

In the last seven years, the young researchers within the ETSF - formerly known as NANOQUANTA - have organized an annual Young Researchers' Meeting (YRM), e.g., Modena, Berlin, Jyväskylä. The purpose of these YRMs is to bring together Ph.D. students and postdocs working on the theoretical and computational aspects of electronic and optical properties of materials within the network.

The YRM 2011, organized by the San Sebastian node, will be the 8th of a series of annual international conferences and the 1st to be held and co-organized outside the ETSF nodes. Specifically, it will be hosted by the University of Naples Federico II. The main aim is to spread the professionalism, knowledge and opportunities from the ETSF to other academic and research realities in Europe and eventually new collaborations.

The meeting constitutes a forum for young researchers who work on various projects within ETSF nodes on the theory and code development. Moreover, it facilitates an open exchange of ideas and various competences and gives an excellent opportunity for future collaborations.

The peculiarity of the YRM is that it is organized and attended solely by young researchers having non-permanent contracts, like postdocs and PhD students. The absence of senior scientists opens further channels for discussion about details and introductory aspects which are typically not covered in a usual meeting. In order to facilitate the interaction between young researchers, plenty of question/discussion time will be reserved. For these reasons we strongly recommend to the youngest participants to contribute with talks and posters.





**Monday**

**16th May 2011**

**20:30 Welcome Party**

**Tuesday**

**May 17th 2011**

**09:00 Welcome**

## **DFT I**

**09:30 Keynote Talk:** F. Eich

From  $v$  to  $n$  and back - An Introduction to Density-Functional Theories

**10:15** T. Baldsiefen

Self-consistent minimization procedure in the theoretical framework of reduced density matrix functional theory (RDMFT)

**10:40-11:15 Coffee Break**

## **DFT II**

**11:15** J. Hashemi

Time Evolution of Density Matrix Using BBGKY Hierarchy

**11:40** F. Agostini

Maximum probability basins for the analysis of atomic densities

**12:05** A. Crawford Uranga

Non-adiabatic contributions to the spectrum of simple molecular models: the case of the one-dimensional dihydrogen cation

**12:30-13:00 Discussion**

**13:00-15:00 Lunch**

## **DFT III**

**15:00** J. Wieferink

Localized resolution of identity for efficient Hartree-Fock exchange, based on numeric atomic orbitals

**15:25** M. Hieckel

Density functional theory study of LO-TO splitting of vibrational modes of insulating compounds

**15:50-16:20 Coffee Break**

## **DFT IV**

**16:20** V. Parente

Spin connection and boundary states in a topological insulator

**16:45** M. Vörös

Calculation of impact ionization rates in silicon nanocrystals using density functional theory

**17:10** L. Matthes

Graphene Superlattices Studied by Ab-Initio Methods

**17:35-19:30** Poster Session

**Wednesday**

**May 18th 2011**

## **TDDFT I**

**09:30 Keynote Talk:** L. Caramella

Theoretical spectroscopy of realistic systems

**10:15** J. Ramsden

Intrinsic memory effects in the exact time-dependent Kohn-Sham potential

**10:40-11:15** Coffee Break

## **TDDFT II**

**11:15** D. Kammerlander

Optimal Control of the Electronic Current Density

**11:40** J. Walkenhorst

Modelling Inelastic Electron Tunnelling with TDDFT - Bugs and Features

**12:05** M. Bertocchi

The optical properties of Si/CaF<sub>2</sub> multi-quantum wells: role of size and interface configuration

**12:30-13:00** Discussion

**13:00-15:00** Lunch

## **TDDFT III**

**15:00** R. Guerra

Interacting Nanocrystals in Si/SiO<sub>2</sub> Systems: From Quantum Dots to Quantum Networks.

**15:25-16:10 Scientific Topic:** L. Stella

Chemical accuracy by throwing random numbers? A brief introduction to Quantum Monte Carlo methods

**16:10-16:40** Discussion

**16:40-17:10** Coffee Break

**20:30** Social Dinner

**Green's functions and GW**

**10:00 Keynote Talk:** F. Caruso

The GW approximation of the many-body problem: from perturbative  $G_0W_0$  to full self-consistency

**10:45** M.C.T.D. Müller

T-matrix approach for electron-magnon interactions in ferromagnetic materials

**11:10 - 11:45 Coffee Break**

**Spectroscopy**

**11:45** U. De Giovannini

Photo-electron spectroscopy with TDDFT

**12:10** M. Guzzo

Satellites in Photoemission Spectroscopy

**12:35** M. Govoni

Auger Recombination in Si and GaAs from first-principles

**13:10-13:30 Discussion**

**13:30-15:00 Lunch**

**Applications: ZnO I**

**15:00** G. Antonius

Pushing  $G_0W_0$  limits with ZnO

**15:25** Y. Xu

First-principles study of the ZnO/organic interface: the relation between surface structure and interface properties

**15:50-16:20 Coffee Break**

**Applications: ZnO II**

**16:20** R. D'Amico

First-principles calculations of clean and defected ZnO surfaces

**16:45-17:15 Discussion**

## Biosystems

**09:30 Keynote Talk:** M. Wanko

Computational Approaches for Complex Systems

**10:15** L.A. Espinosa Leal

Toward a unified real-time real-space description of Magneto Optical response in closed-shell molecular systems

**10:40** G. Tahereh

A TDDFT Study of Guanine-Cytosine base pairs in Watson-Crick and Hoogsteen configuration

**11:05-11:35 Coffee Break**

## MC and strong correlations

**11:35** D. Karlsson

A TDDFT approach for the 3D Hubbard model in the linear and non-linear regime

**12:00** N. Slama

Approximations for Green's functions calculations from the Hubbard Molecule

**12:25-12:55 Discussion and Farewell**

# Oral Contributions

# From v to n and back - An Introduction to Density-Functional Theories

F. G. Eich

*1 Institut für theoretische Physik, Freie Universität Berlin, Arnimallee 14, Berlin, Germany*

*2 Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle, Germany*

*3 ETSF*

Density-Functional Theory and its offspring are widely used when one aims at the description of interacting particles. Furthermore Density-Functional Theories serve as starting point for other approaches to the many-body problem, e.g. self-consistent Many-Body-Perturbation Theory [1]. In the hope of setting the stage for more specialized talks, we will present the fundamental ideas and concepts of Density-Functional Theories. Starting with a discussion of the seminal Hohenberg-Kohn theorem and its ramifications [2], we will focus on the application of Density-Functional Theories to the determination of the ground-state energy. The Kohn-Sham scheme [3], a tool for obtaining the ground-state energy, and its (un)-physical interpretation will be reviewed, comparing plain-vanilla Density-Functional Theory and Reduced-Density-Matrix-Functional Theory [4]. Finally we will revisit the Local-Density Approximation to the exchange-correlation energy and present possible generalizations.

[1] L. Hedin, Phys. Rev. 139, A796 (1965)

[2] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964)

[3] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965)

[4] T. L. Gilbert, Phys. Rev. B 12, 2111 (1975)

## Self-consistent minimization procedure in the theoretical framework of reduced density matrix functional theory (RDMFT)

T. Baldsiefen

*Max-Planck-Institut Halle/Germany*

As a close relative to DFT, RDMFT proved to be successful on some fields of research where DFT struggles [1,2]. We will show, that against prevalent beliefs it is possible to construct a Kohn-Sham-like system in RDMFT and use it in a self-consistent minimization scheme.

[1] Sharma et al., PRB 78, 201103 Rapid Comm. (2008)

[2] Lathiotakis et al., PRA 79, 040501 (2009)

## Time Evolution of Density Matrix Using BBGKY Hierarchy

A. Akbari<sup>1</sup>, M.J. Hashemi<sup>2</sup>, R. Van Leeuwen<sup>3</sup>

*1 Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco, San Sebastián, Spain*

*2 Department of Applied Physics, Aalto University, P.O. Box 11100, FI-00076 AALTO, Finland*

*3 Department of Physics, Nanoscience Center, FIN 40014, University of Jyväskylä, Jyväskylä, Finland*

Our work starts with the BBGKY hierarchy equations which can be straightforwardly derived from the time-dependent Schrödinger equation for the reduced density matrices, RDM's. As in all hierarchical formalisms, BBGKY equations couple a RDM of a given order to the one-order-higher RDM. In order to make this set of equations tractable we need to truncate the hierarchy.

The first two equations of the hierarchy read

$$\begin{aligned} & \left( i\partial_t - \hat{h}(\mathbf{x}_1, t) + \hat{h}(\mathbf{x}'_1, t) \right) \gamma(\mathbf{x}_1, \mathbf{x}'_1, t) \\ & = \int d\mathbf{x}_2 (U(|\mathbf{r}_1 - \mathbf{r}_2|) - U(|\mathbf{r}'_1 - \mathbf{r}_2|)) \Gamma(\mathbf{x}_1 \mathbf{x}_2; \mathbf{x}'_1 \mathbf{x}_2, t) \end{aligned}$$

and

$$\begin{aligned} & \left( i\partial_t - \hat{H}_{12} + \hat{H}_{1'2'} \right) \Gamma(\mathbf{x}_1 \mathbf{x}_2; \mathbf{x}'_1 \mathbf{x}'_2, t) \\ & = \sum_{i=1}^2 \int d\mathbf{x}_3 (U(|\mathbf{r}_i - \mathbf{r}_3|) - U(|\mathbf{r}'_i - \mathbf{r}_3|)) \Gamma^3(\mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3; \mathbf{x}'_1 \mathbf{x}'_2 \mathbf{x}'_3, t), \end{aligned}$$

where  $U(12)$ ,  $\hat{h}_1$  and  $\hat{H}_{12}$  are interaction between particles, one- and two-body Hamiltonians while  $\gamma, \Gamma$  and  $\Gamma^3$  are one-, two- and three-body RDM respectively.

Here, we truncate the hierarchy at the level of second equation by approximating  $\Gamma^3$  in terms of  $\gamma$  and  $\Gamma$ . The quality and stability of different approximations will be investigated.

## MAXIMUM PROBABILITY BASINS FOR THE ANALYSIS OF ATOMIC DENSITIES

F. Agostini

*Max-Planck-Institut fuer Mikrostrukturphysik, Halle (Germany)*

Tridimensional atomic densities, firstly introduced by P.G. Kusalik [1], are frequently used as a tool to investigate the structure in disordered systems as liquids. The representation in 3D space of such densities gives a complete picture of the short-range order of the liquid around a fixed molecule, beyond the information usually obtained by the computation of the radial distribution function [2]. However, in general only a qualitative description of the structure of liquids is extracted by the analysis of this atomic densities. The aim of this work is developing a technique which goes beyond a purely qualitative analysis of the tridimensional atomic densities in a liquid and proposing the calculation of suitable quantities which characterize such structure. The proposed method is a generalization, to a classical (disordered) system, of the method developed by A. Savin and coworkers [3] to localize opposite-spin electron pairs in 3D space. The fundamental quantity which characterizes the localization in space of particles is the probability of finding one and one particle in a region of space  $\omega$ . The probability is calculated by spatial integration of a probability density, which is represented, for a N-electron system, by the squared modulus of the electronic wavefunction. In the proposed classical generalization, such probability density is the microscopic (canonical) density in configuration space, and the probability is sampled over a molecular dynamics trajectory. The optimization of  $\omega$  in order to maximize this probability is the key operation used to identify the region of space where it is more likely to find one and only one particle. The level set method [4,5] is used to achieve this optimization, by determining the evolution equation, in a fictitious time variable, of the border of  $\omega$ . Some applications of this method will be described, by presenting some results from the analysis of the solvation structure of water around a water molecule. The connection between these results and the usual picture in terms of solvation shells will be presented, together with some analysis of the population dynamics in the optimized  $\omega$ 's.

[1] P.G. Kusalik and I.M. Svishchev. *Science* 265 1219 (1994)

[2] J.P. Hansen and I.R. McDonald. *Theory of simple liquids*, Elsevier Ltd., II edition (1986)

[3] A. Scemama, M. Caarel and A. Savin. *J. Comput. Chem.* 28 442 (2007)

[4] S. Osher and F. Santosa. *J. Comput. Phys.* 171 272 (2001)

[5] S. Osher and J.A. Sethian. *J. Comput. Phys.* 79 12 (1988)

## Non-adiabatic contributions to the spectrum of simple molecular models: the case of the one-dimensional dihydrogen cation

A. Crawford Uranga

*Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, San Sebastián, Spain*

The optical spectra calculated from linear response and real-time propagation Time-Dependent Density Functional Theory (TDDFT) provide a good approximation to the true spectra. However, there are situations in which current adiabatic functionals are not accurate enough. In particular, within the adiabatic approximation, the history-dependent part of the electron-nuclear interaction cannot be properly modelled. In the present work, we have compared results from the exact diagonalisation and the Born Oppenheimer Approximation (BOA) of the time propagation of a one-dimensional model of the dihydrogen cation (the real-space code Octopus [1] has been used for this purpose), to quantify non-adiabatic contributions to its optical spectra. In particular, we assess the accuracy of the BOA by fictitiously varying the proton mass. The numerical analysis employed in this preliminary investigation can be extended to a one-dimensional model of the hydrogen molecule to include electron-electron correlation effects. We think that the physical insights gained studying these simple model systems might help understanding more complex non-adiabatic processes, such as molecular photodissociation by attosecond laser pulses [2].

[1] <http://www.tddft.org/programs/octopus/wiki/index.php/Main> page

[2] Sansone et al. Nature 465 7299 (2010)

## Localized resolution of identity for efficient Hartree-Fock exchange, based on numeric atomic orbitals

J. Wieferink

*Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin*

Methods based on an exact exchange operator (EX) are increasingly popular, but are still restricted to analytical basis functions (e. g. Gaussians) for medium system sizes. We here introduce a localized resolution-of-identity approach for the two-electron Coulomb operator, based on expanding single-particle basis function products separately into auxiliary atom-centered basis sets that are restricted to two centers. Our approach produces accurate results for all-electron EX, can be applied both to analytical and numeric basis functions, requires only  $O(N^2)$  intermediate storage and retains a path towards  $O(N)$  EX for large systems. We demonstrate a total-energy accuracy of  $\pm 1$  meV/atom with a good error cancellation in binding energies for systems including S22 benchmark molecule set [1], using the numeric atom-centered orbital based all-electron electronic structure code FHI-aims [2].

[1] P. Jurecka et al., Phys. Chem. Chem. Phys. 8, 1985 (2006).

[2] V. Blum et al., Comput. Phys. Comm. 180, 2175 (2009).

## Density functional theory study of LO-TO splitting of vibrational modes of insulating compounds

M. Hieckel, D. Reith, R. Podloucky

*Faculty for Chemistry, Univ. Vienna*

We present results of density functional theory (DFT) calculations for vibrational properties of insulating compounds derived by the force constant method [1]. For the exchange-correlation functional the generalized

gradient approximation as well as a hybrid functional were used. The LO-TO splitting in ionic solids is due to the long range Coulomb interactions which is caused by the coupling of atomic displacements to the thus generated electrostatic field [2]. The modelling is based on an additional nonanalytic term to the dynamical matrix which depends on the Born effective charges and the dielectric constant whose tensors are derived from DFT calculations of the macroscopic electronic polarization [3]. The results for nonmagnetic ionic compounds are as well as for the transition metal oxides MnO and NiO are presented and compared to experiment.

[1] D. Reith, program package fPHON based on PHON by D. Alfè, 1998.

[2] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices*, Oxford University Press, 1954.

[3] R.W. Nunes and X. Gonze, Xavier, *Phys. Rev. B* **63**, 155107 (2001).

## Spin connection and boundary states in a topological insulator

V. Parente

*Università degli Studi di Napoli "Federico II"*

We study the surface resistivity of a three-dimensional topological insulator when the boundaries exhibit a non trivial curvature. We obtain an analytical solution for a spherical topological insulator, and we show that a non trivial quantum spin connection emerges from the three dimensional band structure. We analyze the effect of the spin connection on the scattering by a bump on a flat surface. Quantum effects induced by the geometry lead to resonances when the electron wavelength is comparable to the size of the bump.

## Calculation of impact ionization rates in silicon nanocrystals using density functional theory

M. Vörös

*Budapest University of Technology and Economics*

Multi exciton generation in nanocrystals is considered to be one of the possible candidates to overcome the well-known Shockley-Queisser limit in semiconductor solar cells. A theoretical understanding of the experiments is still missing and could significantly contribute to the debate in the field. In the literature several different theoretical and numerical studies addressed this problem, mostly supporting the impact ionization mechanism. In previous calculations the impact ionization rates were evaluated for nanocrystals by using empirical pseudopotentials fitted to bulk properties or tight-binding wavefunctions. We present an ab-initio scheme based on density functional theory in a plane-wave pseudopotential implementation that includes static screening at the random-phase approximation level. We will discuss how impact ionization rates are affected by the size and surface properties of small silicon nanocrystals.

## Graphene Superlattices Studied by Ab-Initio Methods

Lars Matthes<sup>1,2</sup>, Karsten Hannewald<sup>1</sup>, Juergen Furthmuellers<sup>1</sup>, Friedhelm Bechstedts<sup>1</sup>

*1 Institut für Festkörpertheorie und -optik, 07743 Jena, Germany*

*2 Dipartimento di Fisica, Università di Roma Tor Vergata, 00133 Roma, Italy*

The peculiar electronic properties of graphene have stimulated extensive research towards graphene-based electronics (for a recent review, see [1]). Hereby, of particular interest are quasi-1D structures such as graphene nanoribbons [2] or, more recently, graphene superlattices [3] which allow a systematic tuning of the band

structure. An impressive example for such modifications has been predicted by recent Kronig-Penney-type calculations [3] for a single graphene layer subject to a 1D periodic potential where a rather counterintuitive anisotropic renormalization of the Fermi velocity due to the Klein paradox is expected. Here, 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 [4]. 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.

References:

- [1] A.H. Castro Neto et al., Rev. Mod. Phys. 81, 109 (2009)
- [2] See, e.g., U. Treske, F. Ortmann, B. Oetzel, K. Hannewald, F. Bechstedt, phys. stat. sol. (a) 207, 304 (2010)
- [3] C-H. Park et al., Nature Phys. 4, 213 (2008)
- [4] L. Matthes, K. Hannewald, J. Furthmüller, and F. Bechstedt (unpublished)

## Theoretical Spectroscopy of Realistic Systems

L. Caramella

*Universita' degli Studi di Milano*

Spectroscopy is an important experimental technique used to investigate structural, electronic and optical properties of condensed matter systems. An external perturbing field excites the sample and from the response of the system a spectrum is detected containing a number of physical information. Theoretical methods are very helpful in decoding and interpreting such spectra but excitations are complex and dynamical processes are making the ab initio computation very demanding and sometime unfeasible, in particular for real systems. Time dependent density functional theory is the most popular approach able to describe efficiently physical properties of a system. Within this scheme, the many body problem can be treated at different levels of accuracy through appropriate approximations. We will review the theoretical framework and its application to excited states calculations distinguishing the cases of infinite, semi-infinite and finite systems.

## Intrinsic memory effects in the exact time-dependent Kohn-Sham potential

J. Ramsden

*University of York*

Density functional theory (DFT), time-dependent DFT (TDDFT) and current DFT (CDFT) have proven to be powerful tools for calculating electronic properties of systems, for instance the ground state electronic structure, time-dependent responses to perturbations, including magnetic fields, and excitation spectra. Each DFT is in principle an exact reformulation of quantum mechanics in terms of some universal density (or current-density) functional. As yet, this functional is unknown and must be approximated, typically with local density dependence (LDA), or its time-dependent analogue (adiabatic LDA), although the universal functional is known to be non-local. Ultimately, all difficulties in employing DFTs to describe real systems lie in the shortcomings of the approximations used (e.g. band gap errors in semiconductors, binding energies in finite systems). We present results of bottom-up studies of the nature of the exact potential in the Kohn-Sham formalisms of TDDFT and CDFT for exactly-solvable systems described by a non-local potential. These indicate that the exact Kohn-Sham potential is not only non-local in space, but is necessarily time-dependent even in the case of homogeneous steady-state systems. For this to be true, the Kohn-Sham potential must

carry intrinsic memory-effects, independent of the energy-dependence of the potential in the real system. The exact potential demonstrates similarity with those for explicitly time-dependent, inhomogeneous systems, also presented here. The exact density functional dependence of the exact Kohn-Sham potential is suggested to be indirect, with the explicit nature of the potential being to reproduce the correct local band structure of a moving electron subject to a (non-physical) applied bias.

## Optimal Control of the Electronic Current Density

D. Kammerlander

*LPMCN Université Lyon 1*

Quantum optimal control theory [1] is a powerful tool for engineering quantum systems subject to external fields such as the ones created by intense lasers. The formulation relies on a suitable definition for a target functional, that translates the intended physical objective to a mathematical form. We propose the use of target functionals defined in terms of the one-particle density and its current [2]. A strong motivation for this is the possibility of using time-dependent density-functional theory for the description of the system dynamics. We exemplify this idea by defining an objective functional that on one hand attempts a large overlap with a target density and on the other hand minimizes the current. The latter requirement leads to optimized states with increased stability, which we prove with a few examples of one- and two-dimensional one-electron systems.

[1] C. Brif, R. Chakraborti, and H. Rabitz, *New Journal of Phys.* 12, 075008 (2010)

[2] D. Kammerlander, A. Castro, M.A.L. Marques, arXiv:1101.1429v3, accepted in *Phys. Rev. A*.

## Modelling Inelastic Electron Tunnelling with TDDFT - Bugs and Features

Jessica Walkenhorst<sup>1</sup>, Marius Wanko<sup>1</sup>, Alberto Castro<sup>2</sup>, Angel Rubio<sup>1</sup>

*1 NanoBio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC San Sebastián, Spain*

*2 Institute for Biocomputation and Physics of Complex Systems (BIFI), University of Zaragoza, Spain*

Scanning Tunnelling Microscopy (STM) is a widely used experimental tool to investigate the electronic structure of molecules on surfaces. On the theoretical side, time-dependent density functional theory (TDDFT) has become a popular tool to describe and predict electronic properties of materials and, in combination with e.g. Ehrenfest molecular dynamics, to describe the coupling of the electronic system to the ionic degrees of freedom. Modelling electron tunnelling in a non-perturbative way is a major challenge. We demonstrate two different approaches based on TDDFT and discuss their advantages and disadvantages. Furthermore, we discuss the physical and computational pitfalls of describing STM, and charge transfer processes in general, in a TDDFT framework. We point out some special precautions that have to be undertaken while working with a real space TDDFT code.

## The optical properties of Si/CaF<sub>2</sub> multi-quantum wells: role of size and interface configuration

Matteo Bertocchi<sup>1,2,3,4</sup>, Eleonora Luppi<sup>3,4</sup>, Elena Degoli<sup>5,2</sup>, Valerie Veniard<sup>3,4</sup>, Stefano Ossicini<sup>5,2</sup>

*1 Dipartimento di Fisica, Università degli studi di Modena e Reggio Emilia, 41125 Modena, Italy*

*2 CNR - Istituto di Nanoscienze, via Campi 213/A, 41125 Modena, Italy*

*3 LSI-Ecole Polytechnique, CNRS-CEA, 91128 Palaiseau, France*

*4 European Theoretical Spectroscopy Facility (ETSF), Modena Associate Node*

*5 Dipartimento di Scienze e Metodi dell'Ingegneria and Centro Interdipartimentale En&Tech, Università degli studi di Modena e Reggio Emilia, 42122 Reggio Emilia, Italy*

We present an ab-initio study of the linear and the non-linear optical properties of the Si/CaF<sub>2</sub> multi quantum-well, focusing on how different structures influence its optical properties. We perform the calculations varying the quantum confinement of the Si layer and the configurations of the interface between the two materials Si and CaF<sub>2</sub>. For the linear properties, we calculate the dielectric function  $\epsilon$  considering both the independent particle approximation (IPA) and the local fields effects in the random phase approximation (RPA), in order to estimate the importance of the anisotropies at the interfaces. For the non-linear properties, we calculate  $\chi^{(2)}$  for Second-Harmonic Generation (SHG) spectroscopy in IPA and RPA as obtained from the formalism developed in Ref. [1]. Actually the experimental literature describes many possible interface configurations, without any conclusive result. Our theoretical calculations can be compared with the experimental measured SHG spectrum in order to obtain information about the real geometry of the interface.

[1] E. Luppi and H. Hübener and V. Vénierd, Phys. Rev. B **82**, 235201 (2010).

## Interacting Nanocrystals in Si/SiO<sub>2</sub> Systems: From Quantum Dots to Quantum Networks.

R. Guerra

*Università di Modena e Reggio Emilia*

Highly promising results have been obtained in the last years from Si nanocrystals (NCs) in many fields, among which photonics, non volatile memories, and biological applications, while trial photovoltaic devices are under investigation. In all the cases, the main advantage of this system comes from the chance of tuning the optical response by changing the NC size and other structural properties. Evidence of an interaction mechanism operating between NCs has been frequently reported, sometimes indicated as an active process for optical emission, and sometimes even exploited as a probing technique. This interaction has been widely interpreted in terms of a kind of excitonic hopping or migration between NCs, although only more recently the mechanisms for carrier transfer among Si-NCs have been more clearly elucidated. Roughly speaking, the possibility of charge migration reduces the quantum-confinement (QC) effect, possibly leading to the formation of miniband with indirect gaps. It should be noted that, contrary to photonics applications, for photovoltaics purposes the indirect nature of the energy bandgap in Si-NCs is advantageous, since the photogenerated electron-hole pair has a longer lifetime with respect to direct bandgap materials. Therefore, the NC-NC interaction can be considered as an additional parameter (tunable by the NC-NC separation) that contributes to the characterization of the system behavior: while the NC-size primarily determines the absorption/emission energy, the interaction level affects the absorption/emission rates. This picture opens to the possibility of creating from one side (high rates) extremely efficient Si-based emitters (lasers), and from the other side (low rates) photovoltaic devices capable of harvesting the full solar energy with high yields. While the role of the NC size has been extensively investigated by many works, as theoretically like as experimentally, the study of the effects of NC-NC interplay is still at an early stage, due to the difficulties encountered by both the experimental and theoretical approaches. By using DFT-based calculations we

present a detailed analysis about the role of NC-NC interaction in Si-NCs. Our preliminary results indicate that a close packing of the NCs is required in order to have an influence of the interaction mechanism on the QC. In this case the optical absorption in the visible-range is increased beside the exciton lifetime, possibly leading to enhanced photovoltaic characteristics. Moreover, we report the possibility of spatially separating the electron-hole wavefunctions by proper conditions of the neighboring NCs, evidencing additional mechanisms that give rise to deviations from the pure QC picture.

## Chemical accuracy by throwing random numbers? A brief introduction to Quantum Monte Carlo methods

Lorenzo Stella, Claudio Attaccalite, Angel Rubio

*Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, San Sebastián, Spain*

This talk is intended as a first introduction to Quantum Monte Carlo (QMC) methods for electronic structure calculations. Assuming the audience to be fairly acquainted with Density Functional Theory (DFT) calculations, the differences (and similarities) between deterministic methods, like DFT, and QMC have been stressed. In particular, the somehow surprising effectiveness of stochastic methods like QMC is addressed, and the key role of the Metropolis algorithm is elucidated. In the second part of the talk, we give a quick overview of the three most popular QMC methods for electronic structure calculations, namely, the Variational Monte Carlo (VMC), the Diffusion Monte Carlo (DMC), and the Path-Integral Monte Carlo (PIMC). Examples considered in this talk, especially in the VMC part, are mostly taken from the authors' work on the metal-to-insulator crossover of a homogeneous hydrogen chain.

## The $GW$ approximation of the many-body problem: from perturbative $G_0W_0$ to full self-consistency

Fabio Caruso<sup>1,2,3</sup>, Xinguo Ren<sup>1,2</sup>, Patrick Rinke<sup>1,2</sup>, Angel Rubio<sup>1,2,3</sup>, Matthias Scheffler<sup>1,2</sup>

*1 Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany*

*2 European Theoretical Spectroscopy Facility (ETSF)*

*3 Nano-Bio Spectroscopy group, Universidad del País Vasco, Av. Tolosa 72, San Sebastián, Spain  
email: caruso@fhi-berlin.mpg.de*

Based on Green's functions, many-body perturbation theory (MBPT) provides an optimal framework for treating correlation in interacting many-body systems; therefore, it is commonly employed in electronic structure theory to overcome current limitations of single-particle approaches, as density-functional theory (DFT) and Hartree-Fock (HF). For solids, MBPT in the  $GW$  approximation [1] is currently the method of choice for the theoretical description of direct and inverse photoemission experiments. Its application to molecules and nanosystems has been steadily increasing in recent years and an assessment of its performance is emerging. Due to its numerical cost,  $GW$  calculations are mostly performed perturbatively following a DFT or HF calculation, solving the linearized quasi-particle equation. At a higher computational cost, self-consistent  $GW$  ameliorates several shortcomings of the  $G_0W_0$  scheme, such as the violation of particle number conservation and the dependence on the starting point. For small molecules self-consistency substantially improves the description of ionization energies compared to a  $G_0W_0$  calculation based on (semi)local DFT ground states and gives total energies in better agreement with available configuration interaction reference data. This talk will give an introduction into the basic concepts of MBPT and Green's functions, with special focus on the  $GW$  approximation and its application to electronic structure theory. In addition, I will review the different flavours of the  $GW$  approximation such as perturbative  $G_0W_0$ , partially and fully self-consistent  $GW$  schemes, showing achievements and shortcomings of the different methods.

[1] L. Hedin, Phys. Rev. **139**, A796 (1965)

## T-matrix approach for electron-magnon interactions in ferromagnetic materials

M.C.T.D. Mueller

*Peter Grünberg Institut - Forschungszentrum Juelich D 52425 Juelich*

First-principles calculations of the quasiparticle energies and lifetimes in real materials have been performed mainly within the GW approximation (GWA). The GWA has been shown to yield accurate quasiparticle band structures for weakly to moderately correlated systems, whereas it is expected to fail in describing short-range interactions in strongly correlated systems. The scattering between electrons and magnons that takes place in systems with localized d and f orbitals plays an important role in transport and thermodynamic properties of magnetic materials. These scattering phenomena are not accounted for in the GWA. In order to improve the theoretical description of magnetic materials we go beyond the GWA and take higher-order terms into account. We present a formalism that combines the electron-electron scattering described by GWA and the electron-magnon scattering in a unified way. The magnons are calculated with the T-matrix, which describes multiple scattering of electron-hole pairs with different spin. Our implementation is based on the all-electron full-potential linearized augmented-plane-wave (FLAPW) method [1]. As a first step, we calculate the magnon spectra of elementary ferromagnets.

[1] E. Sasioglu, A. Schindlmayr, Ch. Friedrich, F. Freimuth, and S. Blügel, Phys. Rev. B 81, 054434 (2010).

## Photo-electron spectroscopy with TDDFT

U. De Giovannini

*Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, San Sebastián, Spain*

Photo-electron spectroscopy (PES) is a widely used technique to analyze electronic structure of complex systems. The advent of high intense laser sources have extended the range of applicability of this technique to a vast variety of non-linear phenomena like high harmonic generation, above threshold ionization, bond softening and vibrational population trapping. Furthermore, it has turned femtosecond time-resolved pump-probe PES as a powerful technique for the characterization of the excited-state dynamics in nano-structures and biological systems. Here we present a feasible computational procedure to calculate within TDDFT the PES of atoms and molecules excited by short laser pulses. The wave-function is evolved in time and masked above a give radii. This geometrical approach provides a simple description of the energy and angle resolved photo-electron spectrum including multi-photon effects.

## Satellites in Photoemission Spectroscopy

M. Guzzo, M. Gatti, F. Sottile, P. Romaniello, G. Lani, F. Sirotti, J.J. Rehr, L. Reining

*LSI, Ecole Polytechnique, Palaiseau, France*

The *GW* method [1] from Many-Body Perturbation Theory (MBPT) 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 some real materials [3].

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 approximation (CE) for the Green's function, very popular in core-level spectroscopies, has been able to describe satellites correctly also in the case of valence spectroscopy [3], but its theoretical basis has been proved only for models. We obtain the cumulant expansion by means of approximations on the 1-particle Green's function's equation of motion, giving a rigorous derivation for this approximation. We show that the CE gives excellent agreement with experiment. The effectiveness of this approach is going to be tested on more complex systems, such as NiO.

[1] Hedin, L., Phys. Rev. 139 (1965) A796.

[2] Hedin, L., Lundqvist, B.I. and Lundqvist, S., J. Res. Natl. Bur. Stand. Sect. A 74A, 417 (1970)

[3] Aryasetiawan, F., Hedin, L. and Karlsson, K., Phys. Rev. Lett. 77 (1996) 2268.

## Auger Recombination in Si and GaAs from first-principles

M. Govoni <sup>1,3,4</sup>, I. Marri <sup>2,4</sup>, S. Ossicini <sup>2,4</sup>

<sup>1</sup> Dipartimento di Fisica, Università degli studi di Modena e Reggio Emilia, 41125 Modena, Italy

<sup>2</sup> Dipartimento di Scienze e Metodi dell'Ingegneria and Centro Interdipartimentale En&Tech, Università degli studi di Modena e Reggio Emilia, 42122 Reggio Emilia, Italy

<sup>3</sup> CNR - Istituto di Nanoscienze, via Campi 213/A, 41125 Modena, Italy

<sup>4</sup> European Theoretical Spectroscopy Facility (ETSF), Modena Associate Node

Auger Recombination is one of the most important non-radiative recombination mechanisms in semiconductors, as proved both experimentally [1,2] and theoretically [3,4]. Understanding the physics of Auger recombination has crucial practical applications in photovoltaics, namely it represents an important step in the determination of the microscopic parameters that can affect solar cell performances [5]. In this work, we present a first-principle study of the Auger Recombination for n- and p-type Si and GaAs bulk structures. 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 importance of higher order non-radiative recombination mechanisms.

[1] J.Schmidt *et al.*, J. Appl. Phys., **81**, 6186 (1997).

[2] R.Conradt *et al.*, Solid State Commun., **10**, 321 (1972).

[3] K.T.Delaney *et al.*, Appl. Phys. Lett., **94**, 191109 (2009).

[4] S.Picozzi *et al.*, Phys. Rev. Lett., **89**, 197601 (2002).

[5] M.J.Kerr *et al.*, Prog. Photovolt: Res. Appl., **11**, 97 (2003).

## Pushing $G^0W^0$ limits with ZnO.

G. Antonius

*Universite Catholique de Louvain*

Zinc oxide is a wide band gap semiconductor whose technological applications has prompted the theoretical community to find efficient techniques for its numerical description. It has however long been known as a pathological case for  $G^0W^0$  calculations, and many authors still do not agree on the value one should obtain for the band gap with this method. In an attempt to clarify the situation, we review the most common approximations used on the way to obtaining the electronic structure. One such is to rely on a plasmon pole model (PPM) to treat the dynamical dependence of the self-energy. We thus investigate on the performance of various plasmon pole models, such as the Hybertsen-Louie PPM or the Godby-Needs PPM. Their behaviour

on ZnO is compared with a full frequency treatment. Another common practice is to use a Hubbard +U term to account for the correlation among the zinc 3d states. Once again, several ways of applying this model exist, and we show that the final effect of this term on the band gap depends strongly on the fine details of the procedure. Finally, we discuss the pros and cons of the PAW formalism as opposed to the pseudopotential approach, and address some technical issues related to the technique.

## First-principles study of the ZnO/organic interface: the relation between surface structure and interface properties

Y. Xu

*Fritz Haber Institute der MPG, Berlin, Germany*

Hybrid inorganic/organic materials have opened up new opportunities for the development of optoelectronics. Their potential benefit is to combine the best features of two distinct material classes. The understanding of their interfacial properties is of critical importance to develop new basic concepts for optoelectronic devices or to optimize device designs. In this work, we studied the interface between the polar surfaces of zinc oxide (ZnO) and a prototypical organic acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) using first principles approaches implemented in the FHI-aims code [1]. The rich surface phase diagram of the two ZnO polar surfaces (i.e., (0001)-Zn and (000-1)-O) makes the problem complex, but on the other hand offers plenty of room to investigate interfaces with quite different properties. While F4TCNQ binds strongly to the clean ZnO (0001)-Zn surface, only weak physical adsorption is observed on the clean ZnO (000-1)-O surface, where van der Waals interactions play a dominant role. On the reconstructed surfaces, the molecule shows repulsive interactions with surface O adatoms but attractive interactions with surface OH groups. Our results are an important first step to develop a complete understanding of the relation between surface structure and interface properties and may guide the design of hybrid inorganic/organic systems with desired properties.

[1] Volker Blum, Ralf Gehrke, Felix Hanke, Paula Havu, Ville Havu, Xinguo Ren, Karsten Reuter, and Matthias Scheffler, *Computer Physics Communications* 180, 2175-2196 (2009).

## First-principles calculations of clean and defected ZnO surfaces

N.R. D'Amico, D. Ninno, G. Cantele

*CNR-SPIN and Universita' degli Studi di Napoli "Federico II", Dipartimento di Scienze Fisiche  
Compl, Univ. M. S. Angelo, Via Cintia, I-80126 Napoli, Italy*

We carried out a theoretical study of the non – polar ZnO (1010) and ZnO (1120) surfaces using ab initio techniques based on density functional theory. We investigate the effects of both surface and subsurface oxygen vacancies on the structural and electronic properties. We show that the defect formation energy strongly depends on the position of the defect with respect to the surface. Our results imply that subsurface defects could play a major role in the reactivity of the surface. We also perform a first-principles study of the diffusion behaviour of oxygen vacancies in both bulk ZnO and across the above mentioned non polar surfaces. To this end, we derive, with the climbing image nudged elastic band method, the complete set of migration paths for O vacancy diffusion and we find that the oxygen vacancy diffuses much more easily across the surface than in the bulk.

## Computational Approaches for Complex Systems

M . Wanko

*Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, San Sebastián, Spain*

The field of computational physics and chemistry moves towards the simulation of more and more complex systems. On the other hand, the physics of these systems often still involves quantum effects that require an accurate computational model. In order to access the relevant time-scales and system sizes, multi-scale and course-grained approaches are necessary. In this talk I will present techniques and problems involved in the quantum description of large non-periodic systems and their coupling to the environment. Examples will focus on the optical properties of biologic systems.

### Toward a unified real-time real-space description of Magneto Optical response in closed-shell molecular systems

L.A. Espinosa Leal

*Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, San Sebastián, Spain*

We present in this work a newfangled and unified treatment in the real-time real-space for the calculation of the magneto optical response in closed-shell molecular systems. In this approach the classical A and B terms are calculated as an unique term that includes all the electronic transitions stored in the second order term from the expansion coefficients in the magnetically perturbed polarizability. Comparison with the experimental results give a good agreement in small benchmark molecules for the sign of the transition and a fairly agreement with the relative intensities.

### A TDDFT Study of Guanine-Cytosine base pairs in Watson-Crick and Hoogsteen configuration

T. Ghane<sup>1,2</sup> , D. Varsano<sup>1,3</sup>, G. Brancolini<sup>1</sup> , R. Di Felice<sup>1</sup>

*1 Centro S3, CNR Istituto di Nanoscienze , Modena, Italy*

*2 Department of Physics, University of Modena e Reggio Emilia, Modena, Italy*

*3 University of Rome "La Sapienza", Department of Physics, Rome, Italy*

The investigation of the electronic structure and optical properties of DNA and DNA derivatives is of paramount importance in several scientific fields, from nanotechnology to molecular biology and drug design. In this work we study the optical signals of Watson-Crick and Hoogsteen H-bonds that are involved in the triplex formation between protonated Cytosine, Guanine and neutral cytosine. Because optical properties and transfer integrals have a strong dependence on the structure that is selected for the calculations, to bypass this limitation, we perform a Molecular Dynamics simulation to extract significant structure. We apply a clustering to generate meaningful structures from the dynamical trajectories at 300 K, thus taking into account in a simple fashion the conformational variability in the optical spectra. Photo-absorption Spectra compute for the selected structures using the octopus package in the framework of TDDFT in the real-time real-space implementation. We analysis in detail the impact of hydrogen bonding in the calculated spectra for both, Watson-Crick and Hoogsteen conformation.

# A TDDFT approach for the 3D Hubbard model in the linear and non-linear regime

D. Karlsson, C. Verdozzi, M. Puig von Friesen, C.-O. Almbladh, U. von Barth

*Lund University*

Two aspects of TDDFT, the linear response approach and the adiabatic local density approximation, are examined from the perspective of lattice models. We present results for the density response function of the 3D homogeneous Hubbard model, and point out a drawback of the linear response scheme based on the linearized Sham-Schlüter equation. Finally, we analyze the time evolution of the density in a small cubic cluster, and compare exact, adiabatic-TDDFT and Kadanoff-Baym-Equations densities.

## Approximations for Green's functions calculations from the Hubbard Molecule

Nader Slama, G. Lani, P. Romaniello, Lucia Reining.

*Ecole Polytechnique (Palaiseau - France)*

We are interested in understanding the photo-emission process in strongly correlated systems, hence we are trying to give a good description of the spectral function of such class of materials. To date, methods like the GW approximation are employed to this purpose, although they often poorly describe it. In this work, we will employ a model system, namely the Hubbard Molecule (where an exact expressions for the Green's function can be obtained), as a benchmark. We will test different forms of self consistency in the GW Approximation and we will test alternative approximations to calculate the one-body Green's Function.

# Posters

## SiGe Core-Shell Nanowires for Photovoltaics: ab-initio results

M. Amato<sup>1,2</sup>, S. Ossicini<sup>1,2</sup>, R. Rurali<sup>3</sup>

*1 "Centro S3", CNR-Istituto Nanoscienze, Via Campi 213/A, 41125 Modena, Italy;*

*2 Dipartimento di Scienze e Metodi dell'Ingegneria, Centro Interdipartimentale En&Tech, Università di Modena e Reggio Emilia, Via Amendola 2 Pad. Morselli, I-42100 Reggio Emilia, Italy;*

*3 Institut de Ciència de Materials de Barcelona (CSIC), Campus de Bellaterra, 08193 Bellaterra, Barcelona, Spain*

Recently a number of new strategies that may substantially improve the performance and lower the cost of photovoltaics have emerged. In particular much effort has been dedicated to the investigation of electronic properties of pure silicon and pure germanium nanowires (Si and Ge NWs) as promising candidate for building new concept solar energy devices [1,2]. Their photovoltaic application requires a controlled doping and a whole understanding of how electrical properties depend on the doping level of the wire. One of the main limit of doping of pure Si and Ge NWs is its inefficiency when the diameter is reduced, as a consequence of surface segregation of impurities, strong quantum confinement and dielectric mismatch [3-5]. In the case of doping with boron or phosphorus impurities of Si and Ge NWs the impurity state is deep into the band gap and cannot be electrically activated at typical device temperatures. This phenomena is responsible of several problems about the real applications of these types of materials for solar devices. The results of our ab-initio DFT calculations on core-shell silicon-germanium NWs [6] (with diameter of 2.4 nm) show how this limit can be easily overcome by opportune doping with boron and phosphorus impurities [7]. In these nanostructures, infact, the band offset between the two materials causes a localization of the valence states on germanium and of conduction states on silicon [8,9]. As a consequence of this property, with particular doping conditions, a one-dimensional electron (hole) gas at the band edge is created and the carrier density is uniquely controlled by the impurity concentration without no need of thermal activation. In this way, doped SiGe core-shell NWs provide a material ideal suited for photovoltaic applications, since it fulfils two of their fundamental applications, i.e. to separate electrons and holes and to make both carriers electrically active.

[1] T. J. Kempa, et al. *Nano Lett.* **8**, 10, 3456 (2008).

[2] A. Du Pasquier, et al. *Appl. Phys. Lett.* **91**, 183501 (2007).

[3] M. Diarra, Y.-M. Niquet, C. Delerue and G. Allan, *Phys. Rev. B* **75**, 045301 (2007).

[4] M. T. Bjork, et al. *Nat. Nanotech.* **4**, 103 (2008).

[5] Y. M. Niquet, L. Genovese, C. Delerue and T. Deutsch, *Phys. Rev. B*, **81** 161301 (2010).

[6] M. Amato, S. Ossicini and R. Rurali, *Nano Lett.* **11**, 2, 594–598 (2011)

[7] L. J. Lauhon, et al. *Nature (London)* **420**, 57 (2002).

[8] M. Amato, M. Palummo and S. Ossicini, *Phys. Rev. B* **80**, 235333 (2009).

[9] L. Yang, R. N. Musin, X.-Q. Wang, M. Y. Chou, *Phys. Rev. B* **77** 195325 (2008).

## Electronic states of polar and non-polar InN surfaces within the quasiparticle approach

A. Belabbes, F. Bechstedt

*Friedrich-Schiller-Universitaet, Max-Wien-Platz 1, D-07743 Jena, Germany*

DFT provides an incorrect description of the band gap and excited states of InN. The correction of this error is of considerable importance in understanding the surface physics and semiconducting properties of InN. The purpose of this work is to reevaluate the quasiparticle band structure using the novel LDA-1/2 method for the surfaces states of InN. We restrict ourselves to a discussion of the electronic structure of the clean polar and non-polar surfaces. Our calculations allow us to explain the n-type conductivity of polar InN surfaces and the pinning of the Fermi level. The electronic structure of non-polar InN surfaces is found to be very different from that of the polar surface. It shows a semiconducting behavior, but with surfaces

states that energetically overlap with bulk states. Therefore, these findings suggest an absence of electron accumulation on the non-polar InN surfaces. Our results agree with the previous calculations by C. G. Van de Walle and experimental observations by Wu et al, who provided evidence for an unpinned Fermi level at non-polar surfaces. The results have been obtained with low computational effort, similarly to standard LDA calculations, much in contrast to the GW quasiparticle approach.

## Paramagnons of palladium hydride

C. Bersier, P. Buczek, F. Essenberg, A. Ernst, E. K. U. Gross

*MPI Halle*

The electronic properties of magnets and exchange-enhanced paramagnets are strongly influenced by the spin-flip fluctuations. In particular, their important role in the pnictide high-temperature superconductivity has been conjectured. A prerequisite for any qualitative study is the knowledge of spin flip fluctuation spectrum. We compute it resorting to linear response time dependent density functional theory, recently implemented to study complex metals. First we study Pd and PdH. In Pd the spin fluctuations are believed to be detrimental for superconductivity. We find that doping it with H suppresses the spin fluctuations, which might lead to a superconducting transition. In the newly discovered class of pnictide SC the situation is believed to be opposite; spin fluctuation might mediate coupling leading to a superconducting instability. We study their spectrum in BaFe<sub>2</sub>As<sub>2</sub> and YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>. In the non-magnetic phase, a well defined paramagnon peak appears around the momentum which corresponds to the AFM order in the undoped phase. The implications for developing an unconventional superconducting state will be discussed.

## First-principles study (GW+PAW) on new oxynitride phosphors for white LED

B. Bertrand

*Université Catholique de Louvain (UCL) - IMCN - NAPS*

After the original incandescence lamp, after the invasion of compact fluorescent lamps, white-LEDs will be one of the major actor involved in the future generations of eco-friendly light sources. However, with the exception of incandescence lamp, all types of white light source require the use of phosphors. For novel types of white LEDs, an optimal combination of two green- and red-emitting phosphors absorbing partly the blue light from the InGa<sub>N</sub> LED is mandatory to obtain a white light source by post recombination of the light. We have theoretically studied two oxynitride phosphors, one of which is an efficient green phosphor Ba<sub>3</sub>Si<sub>6</sub>O<sub>12</sub>N<sub>2</sub>:Eu developed at the Mitsubishi Chemical Group Science and Technology Research Center, and the other is a bluish-green phosphor Ba<sub>3</sub>Si<sub>6</sub>O<sub>9</sub>N<sub>4</sub>:Eu that exhibits little luminescence at room temperature. Our first-principles results rely on many body perturbation approach (GW+PAW) applied to the two hosts for Europium dopants : Ba<sub>3</sub>Si<sub>6</sub>O<sub>12</sub>N<sub>2</sub> and Ba<sub>3</sub>Si<sub>6</sub>O<sub>9</sub>N<sub>4</sub>. The calculation shows a slightly narrower energy gap for Ba<sub>3</sub>Si<sub>6</sub>O<sub>9</sub>N<sub>4</sub>, that is 0.33 eV. Yet such a result provides precious keys to understand the thermal quenching mechanism, by comparing materials with a similar chemical composition, but different thermal behaviour. As a next step a deeper analysis with Eu-doped models will shed new light onto the relationship between emission/excitation colors from the Europium luminescent centers, and the properties of their complex ligands (dielectric properties, coordination).

## Graphene interfaces for (nano)electronics applications

I. Borriello

*Universita' di Napoli Federico II*

Thanks to its outstanding transport properties, there is an ongoing, intense effort for employing graphene in new generation electronic devices. The two-dimensional structure, amenable to lithographic techniques, made possible single graphene nanoribbon patterning, with defined width and orientation. Nevertheless, edge roughness and defects still represent a limitation to the engineering of the device properties and performances. More recently, new synthesis techniques have allowed the bottom-up fabrication of atomically precise nanoribbons with different size and topology, opening the route to graphene nanostructures with well controlled properties. We employed ab initio study of very narrow graphene nanoribbons chemically immobilized on metallic contacts focusing on the role played by the resulting interface. In particular, the effects of chemical functionalization and energy level alignment will be discussed.

## Applying hybrid-functional and many-body methods to rare earths: a study of Cerium

Marco Casadei<sup>1</sup>, Xinguo Ren<sup>1</sup>, Joachim Paier<sup>2</sup>, Patrick Rinke<sup>1</sup>, Angel Rubio<sup>1,2</sup>, Matthias Scheffler<sup>1</sup>

*1 Fritz-Haber-Institut der MPG (TH), Berlin, Germany*

*2 Humboldt Universitaet (Institut fuer Chemie), Berlin, Germany*

*3 UPV/EHV, San Sebastian (Fisica Materiales), Spain*

The presence of localized, partially occupied  $f$ -electron states dictates many of the peculiar physical properties of rare-earth materials. In particular, the description of the iso-structural  $\alpha$ - $\gamma$  phase transition in Ce metal poses great challenges to density-functional theory (DFT) based approaches since local/semilocal (LDA/GGA) functionals completely fail to produce the phase transition. Here we address this problem by investigating bulk-like Ce clusters of increasing size using hybrid functionals, that incorporate a portion of exact-exchange, and full exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA). This allows us to systematically study the effects of non-local exchange and correlation in this important system. In all clusters we find two stable configurations with different lattice constants and distinct electronic and magnetic properties, resembling the bulk situation. However, all hybrid functionals predict that the high volume phase (linked to the  $\gamma$ -Ce phase) is lower in energy at zero temperature, in contrast to experiment. Decreasing the amount of exact-exchange in the hybrid functional eventually restores the correct phase ordering, at the expense of introducing an adjustable parameter. We show that EX+cRPA – a physically meaningful screening of exact-exchange – achieves the same effect from first principles.

## Ab initio many-body effects in TiSe<sub>2</sub>

M. Cazzaniga, H. Cercellier, C. Monney, P. Aebi, M. Holzmann, G. Onida, and V. Olevano

*Universita' degli Studi di Milano*

TiSe<sub>2</sub> 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.

## GW and beyond approaches to quasiparticle properties in metals

M. Cazzaniga

*Universita' degli Studi di Milano*

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 bandwidth and lifetime of the quasiparticle compared with GW. On the contrary, the inclusion of the vertex also in the self-energy works in the opposite way. Concerning the spectral functions none of the tested approaches is able to significantly improve the position of the plasmon satellite, which remains far from the experimental position. A more detailed analysis suggests that a trend similar to the bandwidth and lifetimes applies also in this case, even if the presence of some exceptions does not allow to draw a definitive conclusion.

## Spin Excitations in Density Functional Theory for Superconductors

F. Essenberger

*Max Planck Institute Halle (Saale)*

In the density functional theory (DFT) approach for superconducting (SC) materials the anomalous density  $\chi$ , is introduced as an extra basic variable. All ground state expectation values then become functionals of the electronic density  $\rho$  as well as  $\chi$ . In the SC Kohn–Sham system the conjugate potential  $\Delta_{xc}$  defined by  $\frac{\delta E_{xc}}{\delta \chi}$  couples to this density  $\chi$  [1]. Currently the perturbation expansion for  $\Delta_{xc}$  includes terms up to first order in the phonon propagator and the static screened Coulomb interaction within the random phase approximation  $w^{\text{RPA}}$  [2]. However for unconventional superconductors this approach fails. One possible reason for this failure is related to the fact that in these materials the Cooper-pairing is mediated by spin excitations [3]. We present a way to include these spin fluctuations and excitations in the framework of SC-DFT. Following the approach of Vignale *et al.* [4] a replacement for  $w^{\text{RPA}}$  is derived. The new effective electron–electron interaction is spin dependent. It includes the contribution of charge fluctuations as well as longitudinal and transverse spin fluctuations.

[1] L. N. Oliveira, E. K. U. Gross, W. Kohn, Phys. Rev. Lett **60**, 23, 2430-2433 (1988)

[2] M. Lueder, Density Functional Theory for Superconductors, A first Principles Approach to the SC Phase, PhD Thesis, (1998)

[3] D. Manske, Theory of Unconventional Superconductors, Springer-Verlag Berlin Heidelberg, (2004)

[4] G. Vignale, K.S. Singwi, Phys. Rev. B **32**, 4, 2156–2166 (1985)

[5] C. A. Kukkonen, A.W. Overhauser, Phys. Rev. B **20**, 2, 550–557, (1979)

## Spin Excitations in Density Functional Theory for Superconductors Surface reconstruction of Si(110)-(16x2): ab initio calculations

E. Ferraro

*European Theoretical Spectroscopy Facility (ETSF) and Dipartimento di Fisica, Università di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Roma, Italy*

The controlled fabrication of quantum structures on surfaces has attracted great attention because of their high potential for applications in nanoelectronics. Among the low-index nonvicinal surfaces of Si, only Si(110) in the (16x2) phase (one of its two primary reconstructions), shows a natural quasi-1D nanowire-like structure, being composed of equally spaced and alternately raised and lowered "stripes" lying along the [112] direction. The ability of these stripes to act as a template for engineering self-assembled quantum wires has been demonstrated for nanowire meshes and stripes of Si, Au and Ag. In spite of this clear potential, Si(110) remains the least understood of all low-index Si surfaces. The reasons are twofold: the experimental difficulty in preparing a clean, defect-free surface, and the theoretical challenge in describing its complicated long-range reconstruction. Here we present ab initio calculations of the total energy for different possible reconstructions. We then focus our attention on a reasonable specific model (Adatoms<sub>2</sub>) and we show the calculated STM images and the result of the RAS in comparison with the ones of Bechstedt and with the experimental ones.

## Organizing broad material searches

H. Glawe, A. Sanna, E.K.U. Gross

*MPI Halle, Germany*

Computationally searching a wide range of materials for physical properties involves large numbers of calculations. In turn, the evaluation and book-keeping imposes a bigger and bigger amount of work on the researcher, while in principle many trivial tasks could be automatized. The present work presents a framework for job surveillance and the detection/correction of trivial errors. This framework abstracts the underlying peculiarities of the HPC cluster used, such as the handling of temporary (scratch) data and parallel jobs from the researcher, making a job runnable with little modifications on many different machines. In turn, more time is left for the actual research.

## Toward the Absorption Spectrum for Brookite TiO<sub>2</sub>

L. Hung

*ETSF Palaiseau*

Titanium dioxide (TiO<sub>2</sub>) is a widely-used material in photocatalysis due to its high catalytic efficiency and absorption in the UV range. It is generally found in one of three crystal structures: rutile, anatase, or brookite. While ground state and optical properties of the rutile and anatase phases have been often studied through experiment and simulation, brookite has only more recently become a phase of interest after experiments showed increased photocatalytic activity in its presence (relative to pure anatase or rutile). However, brookite is both relatively difficult to synthesize experimentally and more expensive to model. Here, we present our ongoing density functional theory and many-body perturbation theory simulations of the brookite form of TiO<sub>2</sub>, with comparison to the electronic structure and optical behavior of the anatase and rutile phases.

## Going beyond ground state calculations on complex model systems: the case of TiO<sub>2</sub>-based materials

A. Iacomino<sup>1</sup>, A. Migani<sup>1</sup>, L. Chiodo<sup>2</sup>, G. Cantele<sup>3</sup>, and A. Rubio<sup>1</sup>

*1 CSIC and Nano-Bio Spectroscopy Group at UPV/EHU, San Sebastián, Spain*

*2 IIT Center for Biomolecular Nanotechnologies, Lecce, Italy*

*3 CNR-SPIN Università degli Studi di Napoli Federico II, Napoli, Italy*

In the last decades the theoreticians of the material properties have been trying to address the study of excited and complex model systems by both developing theoretical methodologies and by implementing advanced codes to afford demanding calculations. One of the main boost to these efforts is given by the relevant social and commercial rebounds of introducing advanced devices in fields like renewable and sustainable energy production. In this work we do show the application of many-body perturbation theories like GW and BSE to TiO<sub>2</sub>-based model systems, from periodic 3D crystals to spatially confined clusters. Beyond accounting for the reliability of the results, we aim to stress and highlight the complexity and manageability of performing such kind of calculations. In fact, TiO<sub>2</sub> is essentially targeted as a prototype photocatalyzer or charge transferrer thus implying the concurrent needs of excited states and complex model systems. We are pleased to entertain discussions about MBPT theoretic and technical issues, connections with the TiO<sub>2</sub> specific cases, applicability and perspective for other model systems.

## Optical properties of tin dioxide: a PAW approach

A. Miglio, M. Stankovski, M. Giantomassi, X. Gonze, G.-M. Rignanese

*Université Catholique de Louvain, Belgium*

SnO<sub>2</sub> belongs to a class of metal-oxides of great industrial interest as they are electrically conductive and optically transparent.

We first address its structural and electronic properties by standard DFT *ab initio* methods, within the PAW approach. We consider the effect of the many-body correction obtained by a single GW iteration ( $G_0W_0$ ) and self-consistent QSGW (Faleev et al. PRB 76, 165106) on the electronic band structure.

We then investigate SnO<sub>2</sub> optical properties. Fully *ab initio* optical spectra can be computed combining DFT ground state calculations with many body perturbation theory (MBPT). To account for the effect of the electron-hole interaction we have to compute the macroscopic dielectric function via the Bethe-Salpeter equation (BSE) formalism.

We perform the calculations via the BSE within the PAW formalism taking advantage of the available k-points interpolation techniques (e.g. maximally localized Wannier functions).

We compare some of the results we obtained with the PAW with all-electron FP-LAPW approach as well as standard norm-conserving pseudopotentials and we also consider the effect of the inclusion of different Sn semi-core states.

## Theoretical spectroscopy of peptides: effects of conformational changes

Elena Molteni<sup>1,2</sup>, Francesco Mazza<sup>1</sup>, Giovanni Onida<sup>1,2</sup>, Guido Tiana<sup>1</sup>

*1 Department of Physics, University of Milan, via Celoria 16, 20133, Milan, Italy,*

*2 European Theoretical Spectroscopy Facility (ETSF),*

*e-mail: elena.molteni@unimi.it*

This work is aimed towards further developments of our presently available ab-initio theoretical spectroscopy tools suitable for studying and understanding correlations between optical spectra and conformational changes in molecules of biological interest, in particular peptides. As a first application, we are focusing on the 83-92 fragment of HIV-1 protease, which is closely related to the 83-93 fragment, known to be involved in the folding and dimerization of this protein.[1,2] Peptides tend to adopt multiple conformations in solution: this can in some cases hinder structural determination based on spectroscopic data, at the same time making peptides an interesting test system for ab initio calculations. For instance, several softwares and methods exist to extract secondary structure information from circular dichroism (CD) spectra, but in general they rely on databases of proteins, and are not suited to peptides.[3] CD is related to the difference in molar extinction between left and right circularly polarized light by chiral media. Therefore, to be able to compute CD, one first has to compute molar extinction itself, that is to say, absorption spectra. After performing classical molecular dynamics (MD) simulations in order to obtain a set of representative conformers of the chosen peptide, we calculated absorption spectra on some of them, at the independent particle, RPA and TDLDA levels. The results show the presence of charge transfer excitations, and their influence on spectral features.

[1] R. A. Broglia, D. Provasi, F. Vasile, G. Ottolina, R. Longhi, and G. Tiana, "A Folding Inhibitor of the HIV-1 Protease", *Proteins* 62, 928 (2006).

[2] G. Verkhivker, G. Tiana, C. Camilloni, D. Provasi, and R. A. Broglia, "Atomistic Simulations of the HIV-1 Protease Folding Inhibition", *Biophys. J.* 95, 550 (2008).

[3] L. Whitmore and B. A. Wallace, "Protein Secondary Structure Analyses from Circular Dichroism Spectroscopy: Methods and Reference Databases", *Biopolymers* 89, 392 (2008).

## Using First-Principles Explicitly Correlated Methods with Medium-sized Polypeptides: How to get converged energy hierarchies?

M. Rossi, V. Blum, X. Ren, M. Scheffler

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany*

Density-functional theory (DFT) with local or semi-local exchange-correlation approximations is known not to account for all many-body effects. Therefore, in order to have benchmark data especially for systems where full non-local correlation (e.g. van der Waals interactions) plays an important role, one needs to resort to higher level methods. When dealing with polypeptides, the system-sizes tend to be large ( 100 atoms). Therefore, it is only feasible to include the many-body correlation effects through perturbative methods like RPA or MP2. However, even these methods are quite computationally expensive and relative energies between different conformers converge very slowly with standard basis sets size. Moreover, these methods also suffer from a large basis sets superposition error (BSSE). In this work, the development of new numeric atom-centered basis sets for use in explicitly correlated calculations is presented. The new basis sets are small and by themselves reduce substantially the BSSE coming from the correlated core of atoms. If used in conjunction with an atomization counterpoise correction, the errors for the S22 data set and different conformations of the alanine dipeptide become negligible. Results for the Ac-Ala<sub>5</sub>-LysH<sup>+</sup> alanine based polypeptide, computed with exact-exchange plus RPA correlation (EX+cRPA) and MP2 are presented and compared to different GGA, meta-GGA, and hybrid exchange-correlation functionals, also including semi-empirical vdW corrections.

## Matricial form of 1-particle Green's function: memory and correlation

L. Sponza

*Ecole Polytechnique (Palaiseau - France)*

The case of one and two electrons in a 1D-box is studied in presence of an external, time-dependent potential. Solutions are obtained in standard quantum-mechanics formalism and in the second quantization scheme making use of one and two point Green's functions. In this elementary situation, memory and correlation effects are investigated along with the effect of some approximation used in MBPT, e.g. , in the cumulant expansion of the one-particle Green's function.

## Quasiparticle band structure calculations. A comparative study between LDA and Meta-GGA functionals

David Waroquiers<sup>1,2</sup>, Aurélien Lherbier<sup>1,2</sup>, Matteo Giantomassi<sup>1,2</sup>, Martin Stankovski<sup>1,2</sup>, Anna Miglio<sup>1,2</sup>, Micael Oliveira<sup>2,3</sup>, Miguel A.L. Marques<sup>2,3</sup>, Gian-Marco Rignanese<sup>1,2</sup>, Xavier Gonze<sup>1,2</sup>

*1 Université Catholique de Louvain, Institute of Condensed Matter and Nanosciences*

*2 European Theoretical Spectroscopy Facility*

*3 Center for Computational Physics, Universidade de Coimbra*

Recently, the Tran-Blaha meta-GGA (MGGA) functional [1] has been reported to provide an improved description of the electronic structure of various semiconducting and insulating systems relative to standard (LDA or GGA) density-functional theory (DFT) calculations [1,2]. This is very promising since the MGGA calculations do not induce a significant increase the computational cost. However, the mechanism of this improvement is still unclear. In particular, except for the bandgap itself, it has not yet been compared to the results obtained using many-body perturbation theory (MBPT). In this work, MBPT calculations are performed starting from both LDA and MGGA ground-state simulations for different bulk materials (Si, Ge, C-diamond, and some oxydes). Both the *G0W0* and quasiparticle self-consistent *GW* (QS*GW*) calculations are considered allowing us to investigate the quality of both the eigenenergies and eigenfunctions provided by LDA and MGGA.

[1] F. Tran and P. Blaha, Phys. Rev. Lett. 102, 226401 (2009).

[2] D. J. Singh, Phys. Rev. 82, 205102 (2010).

# Participants

# List of Participants

- 1. Federica Agostini** ..... **agostini@mpi-halle.de**  
My research activity focuses on the investigation and application of a new method for characterizing the structure of liquid water, to get new and quantitative insights on the organization of the solvation shells of water around water (and ions) and on the "behavior" of the hydrogen-bond network in different thermodynamic conditions. I am also working on the construction of a consistent formulation of non-adiabatic mixed quantum-classical mechanics, in analogy with the (standard) classical and quantum mechanical formulation of mechanics (dynamics and statistical mechanics).
- 2. Michele Amato** ..... **michele.amato@unimore.it**  
We demonstrate by ab initio electronic structure calculations that extremely high efficiency doping can be achieved in coaxial SiGe nanostructures, taking advantage of a fundamental property of this interface: the type-II band offset. Our results strongly support the idea that SiGe core-shell nanowires provide a system ideally suited for high-efficiency photovoltaic applications, since they fulfill two of their fundamental functions, i.e to separate electron and holes and to render both carriers electrically active.
- 3. Gabriel Antonius** ..... **gabriel.antonius@gmail.com**  
I work on several applications of the GW theory. One is the computation of transparent conducting oxides electronic structure. Another one is the calculation of zero-point motion effect on the band gap of insulators.
- 4. Tim Baldsiefen** ..... **tim.baldsiefen@mpi-halle.de**  
We show, that one can construct a noninteracting system in grand canonical equilibrium which is capable of reproducing any physical 1-reduced density matrix to arbitrary accuracy. We then use this to construct a Kohn-Sham minimization scheme and test it for simple systems. Furthermore we show, that the introduction of a temperature-tensor, i.e. a temperature which is orbital dependent, will speed up the convergence of the minimization scheme considerably.
- 5. Abderrezak Belabbes** ..... **abderrezak.belabbes@uni-jena.de**  
Two main reasons can be drawn from our work. (i) From a methodological point of view, demonstrate that the LDA-1/2 approach able to produce an accurate description of the excited-state properties of the InN surfaces and attain a precision similar to that of GW. (ii) From a computational point of view, the LDA-1/2 correction to the eigenenergies is no more demanding on computer resources than the GW method. However, the results have been obtained with low computational effort, similarly to standard LDA calculations, much in contrast to the GW quasiparticle approach. In this work, we restrict ourselves to a discussion of the electronic structure of the clean polar and nonpolar surfaces.
- 6. Christophe Bersier** ..... **flame\_n\_co@hotmail.com**  
I have calculated the spin susceptibility of various paramagnet with the KKR method.
- 7. Matteo Bertocchi** ..... **matteo.bertocchi@unimore.it**  
Study from ab-initio principles of the non-linear optical properties (second-order dielectric susceptibility) of interfaces, surfaces and nanostructures. Development of the code.
- 8. Bruno Bertrand** ..... **bruno.bertrand@uclouvain.be**  
Ab-initio study of materials of industrial interest for LEDs and photovoltaics. Analysis of formal links between particle physics and condensed matter, especially for what concern many body perturbation theories.
- 9. Robert Biele** ..... **treborB@gmx.de**  
Studying thermal and electronic transport of open quantum systems interacting with many environments described by the stochastic Schrödinger equation. This can be applied to thermoelectric material or time-dependent current-density-functional theory for many-particle systems.
- 10. Ivo Borriello** ..... **ivobor@na.infn.it**  
My work is focused on the theoretical characterization of the structural, electronic, and stability properties of organic-semiconductor complexes and interfaces.

- 11. Lucia Caramella** ..... [lucia.caramella@gmail.com](mailto:lucia.caramella@gmail.com)  
 My scientific interests are focused on the application of methods such as linear response theory, density functional theory and its time dependent extension as well as many body perturbation theory to describe real systems. In particular I am interested in ab initio calculations of structural, electronic and optical properties of crystals, molecules and surfaces to simulate spectroscopies such as electron energy loss and high-resolution electron energy loss in reflectance and transmission geometry, surface differential reflectivity and reflectance anisotropy. Moreover I studied metals, magnetic systems and the role of core polarization effects in theoretical spectroscopy.
- 12. Fabio Caruso** ..... [caruso@fhi-berlin.mpg.de](mailto:caruso@fhi-berlin.mpg.de)  
 My research focuses in the field of ab-initio electronic structure calculation based on Green's function methods, with particular attention to post-DFT schemes such as GW, RPA, MP2. My recent work, concern the numerical development and theoretical study of new self-consistent approaches for the computation of Green's functions in the GW approximation.
- 13. Marco Casadei** ..... [casadei@fhi-berlin.mpg.de](mailto:casadei@fhi-berlin.mpg.de)  
 My work is a study of Cerium clusters. Its collocation is on the field of strongly correlated systems. The methods applied are hybrid functionals.
- 14. Marco Cazzaniga** ..... [marco.cazzaniga@unimi.it](mailto:marco.cazzaniga@unimi.it)  
 Ab initio calculation of excited state properties of bulk system and surfaces. Calculations in TDDFT and GW.
- 15. Alison Crawford Uranga** ..... [alisonc1986@gmail.com](mailto:alisonc1986@gmail.com)  
 I am currently involved in the study of non-adiabatic effects on the dynamics of small molecules in the presence of strong laser fields. In particular, I diagonalise exactly the electron-ion Hamiltonian of a one-dimensional model of the dihydrogen cation to assess the limitations of the Born Oppenheimer Approximation.
- 16. Pierluigi Cudazzo** ..... [pierluigi.cudazzo@ehu.es](mailto:pierluigi.cudazzo@ehu.es)
- 17. Roberto D'Amico** ..... [roberto83@na.infn.it](mailto:roberto83@na.infn.it)  
 structural, electronic, and stability properties of oxides.
- 18. Umberto De Giovannini** ..... [umberto.degiovannini@gmail.com](mailto:umberto.degiovannini@gmail.com)  
 TDDFT, photoemission properties of finite systems, non-linear optics, code development, optical and structural properties of dye molecules for dye-sensitized solar cells
- 19. Florian Eich** ..... [feich@mpi-halle.mpg.de](mailto:feich@mpi-halle.mpg.de)  
 Construction of functionals within Density-Functional Theory (DFT) and Reduced-Density-Matrix-Functional Theory (RDMFT). Phases of the uniform electron gas.
- 20. Leonardo Andrés Espinosa Leal** ..... [espinosa.leal@gmail.com](mailto:espinosa.leal@gmail.com)  
 Calculation of the intrinsic and induced Optical properties in Biological systems with Time Dependent Density Functional Theory.
- 21. Frank Essenberg** ..... [essenber@mpi-halle.mpg.de](mailto:essenber@mpi-halle.mpg.de)  
 At the moment I am working on the stuff described in the abstract. But besides the theoretical work also some coding for the PW code is involed.
- 22. Elena Ferraro** ..... [elena.ferraro@roma2.infn.it](mailto:elena.ferraro@roma2.infn.it)  
 Ab initio calculation of optical properties of silicon surface trough density functional theory and GW correction.

- 23. Tahereh Ghane** ..... **tahereh.ghane@unimore.it**  
 We aim at characterizing the optical signals of Watson-Crick and Hoogsteen H-bonds that are involved in the triplex formation between protonated Cytosine, Guanine and neutral cytosine. To do this, we perform time dependent density functional theory (TDDFT) calculations of the optical absorption and circular dichroism spectra of a single triplet plane. We will eventually compare our results to synchrotron radiation CD data measured for single strand, double strand and triplex DNA oligomers (ETSF project with Angel Rubio in Spain and Steen Nielsen in Denmark) to interpret the measurements for unraveling the signature of H-bonds in the CD spectra. The comparison will not be done on individual oligomer spectra but on the principal component analysis: that's why single-triplet calculations are meaningful.
- 24. Henning Glawe**..... **glawe@mpi-halle.mpg.de**  
 I am performing research on superconductivity of solids. Currently, I prepare a broad-scale search for superconductors using our implementation of SCDFE.
- 25. Marco Govoni** ..... **marco.outatime@gmail.com**  
 My work is mainly based on DFT and Many-Body Perturbation Theory (MBPT). So far I used Quantum Espresso and Ab init for DFT and Yambo for MBPT. In order to get Auger rates I needed to merge the two schemes together and thus I have spent a lot of my PhD in implementing new features in Yambo.
- 26. Roberto Guerra** ..... **robguerra@unimore.it**  
 We present bands structure, band offset, recombination rates, and optical absorption spectra of systems containing single or multiple Si/SiO<sub>2</sub> nanocrystals at different spacings. We discuss the results in comparison to recent experimental observations and validated theoretical models.
- 27. Matteo Guzzo** ..... **matteo.guzzo@polytechnique.edu**  
 This is a theoretical study within Many-Body Perturbation theory. We derive analytically new approximations for the 1-particle Green's function and test them on real systems. Our first test bench is bulk Silicon, which is not as obvious as one could think. In fact, it shows a decent amount of correlation effects that cannot be seized by advanced methods such as GW.
- 28. Javad Hashemi** ..... **jha@fyslab.hut.fi**  
 We use BBGKY hierarchy to calculate the time evolution of a system. We need to truncate the hierarchy by an approximation at some level. Quality and stability of different approximation will be studied.
- 29. Marcel Hieckel** ..... **marcel.hieckel@googlemail.com**  
 Ab-initio calculations of phonon dispersions of ionic compounds were considered with the effect of LO-TO-splitting.
- 30. Linda Hung** ..... **linda.hung@polytechnique.edu**  
 I study the electronic and optical properties of photocatalytic materials, such as TiO<sub>2</sub>. I assess the accuracy of various many-body perturbation theory methods (e.g., RPA, BSE, and GW), comparing to experimental results and also predicting new behavior.
- 31. Amilcare Iacomino** ..... **amilcareiacomino@gmail.com**  
 I work on bulk systems, surfaces and nanostructures for applications in the photovoltaic field and in the understanding of heterogeneous photocatalytic processes. My work is based on many-body and time-dependent theories (i.e. GW, BSE and TDDFT). I use several codes (QuantumEspresso, Octopus, Yambo, Abinit, etc).
- 32. David Kammerlander** ..... **david.kammerlander@univ-lyon1.fr**  
 On one hand, I am working on the theory of light-matter-interaction with ultra-short laserpulses. Specifically I am involved in Optimal Control Theory (see the abstract), doing also some implementations in the code OCTOPUS. On the other hand I am interested in defect physics of solids envisioned in a new generation of photovoltaic materials.

- 33. Daniel Karlsson** ..... **daniel.karlsson@teorfys.lu.se**  
I work with Time Dependent Density Functional Theory applied to the Hubbard model, and my work usually consists of a mixture of coding, analyzing results and performing formal calculations.
- 34. Lars Matthes** ..... **Lars.Matthes@uni-jena.de**  
On the one hand my research is about carbon based materials and heterostructures including primarily graphene where I am interested in structural and electronical properties. On the other hand I work on organic materials, in particular their electronical properties and the influence of van der Waals interactions in these systems. I have just started my PhD, so I will focus on DFT and properties of excited systems to calculate optical properties and hopefully can contribute also in the development of this broad field.
- 35. Daniele Meggiolaro** ..... **mjjldany@gmail.com**
- 36. Anna Miglio** ..... **anna.miglio@uclouvain.be**  
I am currently involved in a research project focused on the structural and optical characterization of transparent conducting oxides (TCOs) by ab-initio techniques. I'm dealing mainly with bulk systems, taking into account defects and doping.
- 37. Elena Molteni** ..... **elena.molteni@unimi.it**  
Ab initio calculation of the electronic spectra of peptides. In practice, a combination of classical (= force field) MD to generate conformations, plus ab initio calculations of optical properties on these conformations. Previous experience on classical MD simulations of biomolecules, in collaboration with experimental NMR spectroscopists.
- 38. Adriano Mosca Conte** ..... **Adriano.Mosca.Conte@roma2.infn.it**
- 39. Mathias Christian Thomas David Mueller** ..... **m.c.t.d.mueller@fz-juelich.de**  
We want to calculate the energy dispersion renormalization due to electron-magnon interaction in Nickel from first principles. For this purpose we approximate the electron-magnon interaction by a convolution of the electronic Green function with the T-matrix. This approximation is implemented in the SPEX code (<http://www.flapw.de>).
- 40. Lydia Nemec** ..... **lnemec@fhi-berlin.mpg.de**
- 41. Vincenzo Parente** ..... **parente@na.infn.it**  
Analysis of surface states in topological insulators. Effects of surface rippling to the conductivity.
- 42. James Ramsden** ..... **jdr500@york.ac.uk**  
The purpose of our research is build an idea of what form the exact exchange-correlation potential term in the time-dependent Kohn-Sham equation should take. We start from the simplest exactly-solvable systems and use their time-dependent charge and current densities to reverse-engineer the exact potential required in a Kohn-Sham representation of the same system. By steadily increasing the complexity and realism of the exactly solvable system, we aim to gain an understanding of which physics must be included in a Kohn-Sham description of otherwise unsolvable systems.
- 43. Mariana Rossi** ..... **rossi@fhi-berlin.mpg.de**  
This work focuses on the use of explicitly correlated methods (RPA, MP2) to describe medium-sized polypeptides. I give details about the development of a new numeric atom-centered orbitals basis sets for use in these calculations.
- 44. Nader Slama** ..... **nader.slama@polytechnique.edu**  
We study the Photo-emission and we search Approximations to improve the Green's Function.

**45. Lorenzo Sponza** ..... **lorenzo.sponza@polytechnique.edu**

This work comes from attempts in finding an analytic form of the four-point polarizability starting from a one-particle Green's function expressed as in the cumulant expansion. Memory effects seem to be crucial; an investigation of whether they arise from manybody-interactions or they are present still in the one-particle system, moved us to this work that is still in progress.

**46. Martin Stankovski** ..... **martin.stankovski@uclouvain.be**

**47. Lorenzo Stella** ..... **lorenzo.stella@ehu.es**

My current research is mostly focused on electron-electron and electron-nuclear correlations in small molecules and low-dimensional systems. In particular, I'm involved in: a) Modeling the electron-electron correlation which yields a Mott insulator in 1D systems. 2) Investigating the role of nonadiabatic electron-nuclear interaction in molecular photodissociation. 3) Studying the dynamics of few electrons in strong magnetic field in 2D.

**48. Márton Vörös** ..... **vormar@gmail.com**

As a PhD student, I am involved in the calculation of optical properties of semiconductor nanocrystals. My work on the calculation of impact ionization rates in silicon nanocrystals sheds light on the effect of atomistic details on the decaying process. Though at this level of theory it is hard to compare results with experiments, I still think that these are crucial issues that must be properly taken into account.

**49. Jessica Walkenhorst** ..... **walkenho@gmail.com**

During my diploma thesis I worked on laser-induced non-thermal melting of III-V semiconductors. Currently I am working on a non-perturbative description of electron tunneling. Also I am working on Optimal Control Theory, e.g. for quantum information theory.

**50. Marius Wanko** ..... **marius.wanko@googlemail.com**

My fields of interest are: theoretical biophysics (multiscale QM/MM modelling, photoactive proteins), excited-state nonadiabatic dynamics, and the assessment of quantum-chemical and DFT-based methods for molecular physical applications.

**51. David Waroquiers** ..... **david.waroquiers@uclouvain.be**

My main research is on defects in amorphous silica and their effects on the electronic and optical properties. I am also working on different other topics related to the GW method and other MBPT.

**52. Jürgen Wieferink** ..... **wieferink@fhi-berlin.mpg.de**

I am the coordinator for the development of the part of FHI-aims related to periodic boundary conditions. In particular, I manage our efforts for nonlocal exchange and correlated methods for bulk systems and surfaces.

**53. Yong Xu** ..... **yongxu@fhi-berlin.mpg.de**

We use DFT methods to investigate hybrid inorganic/organic systems for optoelectronic applications. Our study focuses on properties of the inorganic-organic interface, for which an accurate description of van der Waals interactions and level alignment is of significant importance.

# Working fields

## Foundations of Many-Body Theory

Gabriel Antonius  
Tim Baldsiefen  
Matteo Bertocchi  
Bruno Bertrand  
Fabio Caruso  
Marco Casadei  
Marco Cazzaniga  
Florian Eich  
Frank Essenberger  
Matteo Guzzo  
Javad Hashemi  
Daniel Karlsson  
Mathias Christian Thomas David Mueller  
Nader Slama  
Lorenzo Sponza  
David Waroquiers

## Scientific Computing

Federica Agostini  
Tim Baldsiefen  
Matteo Bertocchi  
Fabio Caruso  
Umberto De Giovannini  
Henning Glawe  
Marco Govoni  
Linda Hung  
James Ramsden  
Mariana Rossi  
David Waroquiers  
Jürgen Wieferink

## Phonons and Vibrational Properties

Christophe Bersier  
Alison Crawford Uranga  
Marcel Hieckel  
Vincenzo Parente  
Lorenzo Stella  
Jessica Walkenhorst

## Bulk Systems and Surfaces

Federica Agostini  
Gabriel Antonius  
Abderrezak Belabbes  
Matteo Bertocchi  
Bruno Bertrand  
Ivo Borriello  
Lucia Caramella  
Elena Ferraro  
Marco Govoni  
Roberto Guerra  
Marcel Hieckel  
Linda Hung  
Amilcare Iacomino  
Anna Miglio  
David Waroquiers  
Yong Xu

## Nanostructures and Nanotubes

Michele Amato  
Ivo Borriello  
Marco Casadei  
Leonardo Andrés Espinosa Leal  
Roberto Guerra  
Amilcare Iacomino  
Lars Matthes  
Vincenzo Parente  
Nader Slama  
Márton Vörös

## Biophysics

Leonardo Andrés Espinosa Leal  
Tahereh Ghane  
Elena Molteni  
Mariana Rossi  
Marius Wanko

### **Foundations of TDDFT**

Alison Crawford Uranga  
Umberto De Giovannini  
Florian Eich  
Matteo Guzzo  
Daniel Karlsson  
James Ramsden  
Lorenzo Stella  
Jessica Walkenhorst  
Marius Wanko

### **Photovoltaics**

Michele Amato  
Gabriel Antonius  
Umberto De Giovannini  
Marco Govoni  
Roberto Guerra  
Linda Hung  
Amilcare Iacomino  
Márton Vörös  
Yong Xu

### **Quantum Monte Carlo**

Lorenzo Stella

### **Molecular Transport**

Tahereh Ghane

### **Optimal Control Theory**

David Kammerlander  
Jessica Walkenhorst

Young Researchers' Meeting  
Naples 2011

Supported by:



European Theoretical  
Spectroscopy Facility

