0.1 Report on the 11^{th} Nanoquanta Workshop on Electronic Excitations: A decade of applications of the Bethe-Salpeter Equation

Houffalize (Belgium)

19-22 September 2006

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The workshop gathered 114 participants from leading international groups. There were 39 oral presentations (17 invited speakers and 22 contributed talks) and 30 posters. The workshop allowed the participants to discuss the advances in the theoretical and computational treatment of optical and dielectric spectroscopy in the framework of many-body-perturbation-theory (MBPT).

Invited speakers from leading international groups gave an in-depth overview of current research activities in MBPT (and related fields) and placed recent results into context. Young researchers (Ph.D. students and post-docs) also had the opportunity to present their work (more than half of the oral presentations were given by non-permanent researchers).

A special emphasis was placed on the assessment of ten years of the Bethe-Salpter Equation (BSE) method presenting its achievements and developments [Session I], applications [Session II], advantages and drawbacks in comparison to the more recent developments of time-dependent density-functional theory (TDDFT) [Session IV & V]. Very interesting discussions took place on the complementarity of the two methods and on the future of BSE with respect to TDDFT.

The state-of-the-art implementations of these ab initio methods into existing numerical codes was presented in this meeting. In the same session, an invited speaker described the most recent experimental advances in the field [Session III].

A session was also devoted to the calculation of excited states using Quantum Monte Carlo simulations [Session VI]. Despite the recent advances which have been presented, the method still remains very demanding in terms of computer time.

A series of presentations focused on quantum transport [Session VII] which is an emerging field of computer simulations and whose importance is increasing in the MBPT community. Indeed, the Green's functions formalism at the heart of MBPT is also particularly well suited to describe electronic quantum transport. Currently, it is used both in the Landauer-Büttiker approach and in the non-equilibrium Green's functions (NEGF) theory, also known as Keldysh formalism. Approaches based on TDDFT have also been presented in this session.

A session was devoted to the latest results obtained in the framework of "Optimized Effective Potentiel"(OEP) within density-functional theory [Session VIII]. It was followed by a series of presentations of applications to surfaces and nanostructures [Session IX]. The last session [Session X] focussed on applications of MBPT.

The poster session gave rise to very interesting discussions. Indeed, wide variety of subjects were being presented and the discussions went well beyond these subjects. The meeting provided an informal atmosphere for stimulating discussions between researchers working in this exciting field. New collaborations were initiated following these discussions.

The presentations were collected (a few are still missing) and are available on the conference website. They will be very useful for both the participants and those people in the field that did not have the opportunity to attend the meeting. In particular, the review talks may also be used as a starting point to enter the field.

Program

TUESDAY, 19 September 2006	
SESSION I : Bethe-Salpeter Equation (Chair : Patrick Rinke)	
9:00	Welcome
9:10	Giovanni Onida (30'+10') The Bethe-Salpeter equation and ab-initio calculations: from the first adventure to a well established tool
9:50	Eric Shirley (30'+10') Progress in GW/Bethe-Salpeter Calculations: what do we know, what do we not know?
SESSION II: BSE applications (Chair : Friedhlem Bechstedt)	
11:00	Claudia Ambrosch-Draxl (25'+5') The Bethe Salpeter Equation applied to organic semiconductors: a critical review
11:30	Catalin Spataru (25'+5') Excitons and their radiative lifetime in semiconducting nanotubes
12:00	Olivia Pulci (25'+5') Electronic and Optical properties of surfaces: ab-initio calculations within MBPT and TDDFT approaches
SESSION III : From experiment to codes via theory (Chair : Gian-Marco Rignanese)	
14:30	Simo Huotari (30'+10') Inelastic x-ray scattering in studies of electronic excitations
15:10	Jelena Sjakste (15'+5') Ab initio calculation of the excitonic linewidth due to electron-phonon interaction in semiconductors
15:30	Yann Pouillon (15'+5') Software integration and development within Nanoquanta
POSTER SESSION	

WEDNESDAY, 20 September 2006

SESSION IV: Time-dependent density-functional theory
(Chair : John Rehr)

9:00	Mark Casida (25'+5') Polarization Propagator Corrections to Linear Response Time-Dependent Density-Functional Theory for Molecules with Closed- and Open-Shell Ground States
9:30	Serdar Ogut (25'+5') Is Nano that Different from the Bulk?
10:00	Olena Butriy (15'+5') Electron-nuclear interaction from Time-Dependent Multi-component Density Functional Theory
10:20	Hans-Christian Weissker (15'+5') Dielectric Function of Silicon for Finite Momentum Transfer Signatures of Short-Range Many-Body Effects

SESSION V: TDDFT vs BSE
(Chair : Rodolfo Del Sole)

11:10	Ilya Tokatly (25'+5') Bethe-Salpeter equation from TDDFT perspective: Diagrammatic representation of the exchange-correlation kernel
11:40	Lucia Reining (25'+5') Many-Body Perturbation Theory and Density-Functionalapproaches: successful combinations
12:10	Esa Räsänen (15'+5') Control of electronic currents by laser in quantum rings

SESSION VI: Quantum Monte Carlo
(Chair : Francesco Sottile)

14:30	Claudia Filippi (25'+5') Excitations in (bio)molecules from quantum Monte Carlo
15:00	Paolo Umari (25'+5') Linear and non-linear dielectric response of periodic systems from quantum Monte Carlo

THURSDAY, 21 September 2006	
SESSION VII : Quantum Transport (Part 1) (Chair : Carl-Olof Almbladh)	
9:00	Ralf Gebauer (25’+5’) Quantum kinetic simulations of electron transport in nanosystems
9:30	Stefan Kurth (25’+5’) An Approach to Quantum Transport Using Time-Dependent Density-Functional Theory
10:00	Kristian Thygesen (25’+5’) Non-equilibrium GW approach to electron transport in nanoscale contacts
SESSION VII : Quantum Transport (Part 2) (Chair : Rex Godby)	
11:00	Hector Mera (15’+5’) Non-local self-energies in quantum transport calculations
11:20	Pierre Darancet (15’+5’) GW description of Correlation effects in Quantum transport on real systems
11:40	Peter Bokes (20’+5’) Dynamics of electrons and ab-initio modeling of quantum transport
12:05	Carl-Olof Almbladh (20’+5’) Classical Nuclear Motion in Quantum Transport
SESSION VIII: DFT OEP band gap (Chair : Xavier Gonze)	
14:30	Fabio Della Sala (15’+5’) Kohn Sham gaps, potentials and excitation energies of finite systems using effective exact exchange-correlation potentials
14:50	Myrta Grning (15’+5’) The effect of nonlocality on the band gap within DFT
15:10	Sangeeta Sharma (15’+5’) Non-collinear magnetism within OEP with a view to spin dynamics

SESSION IX: Optical properties applications: surfaces and nanostructures
(Chair : Ludger Wirtz)

16:00	Luis Ramos (20'+5')
	Additional many-body effects in the absorption spectra of Si nanocrystallites
16:25	Federico Iori (15'+5')
	Optical Spectra of doped Silicon Nanocrystals
16:45	Daniele Varsano (15'+5')
	Exciton localisation of quasi 1D systems and optical properties
17:15	Katalin Gaal-Nagy (15'+5')
	Electronical and optical properties of the Si(113)-3x2 ADI surface: An ab initio study
17:35	Andrei Incze (15'+5')
	Ab initio study of optical spectra for oxidized Si(100) surfaces
17:55	Arno Schindlmayr (15'+5')
	Electronic Properties of Point Defects at the GaAs(110) and InP(110) Surfaces

FRIDAY, 22 September 2006

SESSION X : MBPT and GW applications (Part 1)
(Chair : Ulf von Barth)

9:00	Robert van Leuween (30'+10')
	Propagation of the the Kadanoff-Baym equations for many-electron systems
9:40	Pablo Garcia-Gonzales (25'+5')
	Many-body and TDDFT methods for total energy calculations
10:10	Ricardo Gomez-Abal (15'+5')
	An all-electron GW code based on FP-(L)APW+lo: the role of core electrons

SESSION X : MBPT and GW applications (Part 2)
(Chair : Valerio Olevano)

11:00	Martin Stankovski (15'+5')
	Local and non-local vertex corrections in GW for extended and localised systems
11:20	Riad Shaltaf (15'+5')
	First Principle Calculations of Band Offsets of SiO_2 and $ZrSiO_4$ with Silicon
11:40	Vladen Zhukov (15'+5')
	The first-principle LMTO+U+SO+GW+T approach for the calculations of dynamic spin susceptibilities and life-times of excited electron in metals

POSTER SESSION

P01. Hakim Amara
How to identify defects in carbon nanotubes : STM study and vibrational properties

P02. Claudio Attaccalite
Effect of impurities on the optical properties of BN nanotubes

P03. Silvana Botti
Identification of CdSe fullerene-based nanoparticles
from optical spectroscopy calculations

P04. Damien Caliste
A visualisation tool : V_Sim

P05. Giancarlo Cappellini
Electronic excitations of oligoacenes in four different charge states: -1, 0, +1 and +2

P06. Lucia Caramella
Optical properties of oxidized Si(100)(2x2) surface and local
fields contributions on electron energy loss spectrum

P07. Alberto Castro
Time-dependent electron localisation function:
A tool to visualise and analyse ultrafast processes

P08. Marco Cazzaniga
Study of the small-q contribution to the polarizability and the intraband term:
from the jellium to the periodic solid

P09. Letizia Chiodo
Thiol adsorption effects on Au(111) work function

P10. Christoph Friedrich
All-Electron GW Approximation in the Augmented-Plane-Wave Basis-Set Limit

P11. Juergen Furthmueller
Single-particle excitation energies starting from generalized Kohn-Sham schemes

P12. Viviana Garbuio
Excited states of formamide in water

P13. Matteo Gatti
Nonlocality and frequency dependence of effective potentials

P14. Matteo Gatti
Electronic excitations in Vanadium Oxide (VO_2)

P15. Christine Giorgetti
Ab Initio calculations of graphene like systems

P16. Ralf Hambach
Anisotropy in EEL-spectra for large momentum transfer

P17. Paula Havu
Finite Element Implementation of Green's Function Method
for Transport Problems in Nanostructures

P18. Nicole Helbig
Towards a reduced density matrix functional theory for solids

P19. Conor Hogan
Optical properties of the Sb-stabilized GaSb(001) surface

P20. Andrew Morris
Vertex corrections in localised and extended systems

P21. Tapio Rantala
Photoexcitation of Disperse Red 1: Comparison of Approaches

P22. Xinguo Ren
LDA+DMFT computation of the electronic spectrum of NiO

P23. Claudia Roedl
Modifications of BSE Due to Spin Polarization: Antiferromagnetic MnO

P24. Ersoy Sasioglu
Magnetic phase diagram of the Mn-based Heusler alloys from first-principles

P25. Valerie Véniard
Second order harmonic generation in crystalline semiconductors

P26. Claudio Verdozzi
Entanglement in Anderson Nanoclusters

P27. Claudio Verdozzi
Magnetic field effects on optical and transport properties
in InAs/GaAs quantum dots

P28. Matthieu Verstraete
The GW space-time formalism at finite temperatures

P29. Ludger Wirtz
Electronic excitations in hexagonal layered systems (C and BN)

P30. Zeila Zanolli
Ab initio calculation of structural and electronic properties of
InAs and GaAs having wurtzite crystal structure

ABSTRACTS OF PRESENTED PAPERS

Oral presentations

The Bethe-Salpeter equation and ab-initio calculations: from the first adventure to a well established tool

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We briefly review the formalism and the physics of the Bethe-Salpeter equation approach to compute electron-hole interaction effects in excitation spectra. We then describe how the main formulas developed in the seventies by Hanke and Sham started to be integrated with first-principle methods in the last years of the past century, making the link with Hedin's equations and the GW method. We will point out how a few months were sufficient to trigger contributions from several independent groups, and how this was boosting the progresses of the field through competition and collaboration.

Progress in GW/Bethe-Salpeter Calculations: what do we know, what do we not know?

E.L. Shirley

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The past several years, especially the last ten or so, have witnessed considerable progress in Bethe-Salpeter calculations. This progress has been in the two areas, methods and theory. We would like to highlight the progress made at key steps along the way. This survey will start with the milestone work by Hanke, Sham and Rice. Trying to cite much of the representative work (though it may be too hard to identify and cite all of the work), we will point out lessons learned and open questions that remain. Especially of interest should, and will be, what should we do next? Some possible answers to this question will be proposed. Finally, I would like to suggest orbital-less approaches to many aspects of (local) dielectric response in condensed matter systems. A motivation for this type of calculation is its possibly improved scaling with system size to describe local screening effects. One can compare this to traditional methods, which can involve summations over large numbers of occupied and virtual orbitals that stretch long distances across a physical system.

The Bethe Salpeter Equation applied to organic semiconductors: a critical review

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(2) Institut für Materialphysik, University Vienna

The exciton binding energy is a central quantity in the photophysics of semiconductors, intimately related to the probability of radiative mission/absorption and electric-field induced generation of free charge carriers. Hence, for organic semiconductors this quantity is of major interest concerning their technological application in opto-electronic devices. And it had been a long-standing problem, whether the lowest absorption features in polymers are strongly bound excitons or free electron-hole pairs.

To answer this question, the optical properties including excitonic effects have been investigated for a variety of organic molecular crystals and polymers during the last years, where the electron-hole interaction has been included by solving the Bethe-Salpeter equation.

In this talk, it will be shown, how the electron-hole interaction can be tuned, either by dense packing or by the choice of the molecule, since the exciton binding energies are extremely sensitive to the crystalline environment and to the molecular size. Thereby the influence of the three-dimensional crystal versus a one-dimensional chain is addressed for the polymers. Moreover, the dependence of the exciton binding energy on the molecular size is studied for several series of oligomers and compared to those found for the polymers. As last aspect, the influence of the intermolecular interaction on the excitonic effects is investigated by applying hydrostatic pressure, which provides another way of supressing the Coulomb interaction of the electron-hole pair.

Despite the success of the Bethe Salpeter Equation for the puzzling problem concerning the role of excitons in organic semiconductors, a couple of questions remain. Therefore, our results are not only compared to experimental data and surveyed together with other theoretical findings, but we particularly analyze the sensitivity of the results with respect to different approximations applied in the theoretical approaches.

Excitons and their radiative lifetime in semiconducting nanotubes

C. Spataru

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We present ab initio calculation of self-energy and electron-hole interaction (excitonic) effects on the optical spectra of semiconducting single-walled carbon and BN nanotubes. We employed a many-electron Green's function approach that determines both the quasiparticle and optical excitations from first principles. We found important many-electron effects that explain many of the puzzling experimental findings in the optical spectrum of these quasi-one dimensional systems. The calculated optical spectra are in excellent quantitative agreement with measurements, and show prominent features excitonic in nature.

We have also calculated the radiative lifetime of excitons in semiconducting carbon nanotubes. An intrinsic lifetime of the order of 10 ps is computed for the lowest optically active bright excitons. The intrinsic lifetime is however a rapid increasing function of the exciton momentum. Moreover, the electronic structure of the nanotubes dictates the existence of dark excitons nearby in energy to each bright exciton. Both effects strongly influence measured lifetime. Assuming a thermal occupation of bright and dark exciton bands, we find an effective lifetime of the order of 10 ns at room temperature, in good accord with recent experiments.

Electronic and Optical properties of surfaces: ab-initio calculations within MBPT and TDDFT approaches

O. Pulci(1,2)

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The microscopic study of complex systems has nowadays reached a high level of accuracy that allows for a deep understanding of the electronic excitations. Ab-initio descriptions of experiments such as direct or inverse photoemission, optical absorption, electron energy loss, have become possible thanks to the huge progress in the theory and the increased computational power. Charged excitations, as well as neutral excitations, can now be studied within the Many-Body Perturbation Theory (MBPT) based on the Green's function formalism. The so called GW approximation allows to calculate the band structure of solids and surfaces with a very good accuracy. Optical spectra of surfaces can be calculated at different levels of approximation: within single particle schemes (DFT or GW), or including the electron hole interaction within the Bethe Salpeter equation (BSE) or the TDDFT approach. Here we present in details results for band structures, electron affinity, and optical spectra of diamond and silicon surfaces. Several approximations used for computing the electronic band structures and optical spectra will be analized and discussed.

Inelastic x-ray scattering in studies of electronic excitations

S. Huotari

European Synchrotron Radiation Facility (ESRF)

Inelastic x-ray scattering (IXS) is a rapidly developing tool in the studies of excitations in condensed matter. The spectral range covers a multitude of phenomena, from phonons (a few meV) via valence-electron plasmons (a few eV) to core-electron excitations (10 eV to several keV). Basically two different types of experimental setups can be utilized, namely resonant and non-resonant IXS. In resonant IXS, photon energy is tuned to a core level threshold of the target material and several otherwise weak or forbidden excitations can be resonantly enhanced. In non-resonant IXS, the information obtainable is the dynamic structure factor, which is in turn directly related to the macroscopic dielectric function. This technique is closely related to electron energy-loss spectroscopy with certain advantages and disadvantages. These issues will be reviewed and recent developments in synchrotron radiation instrumentation will be discussed in terms of which experiments are feasible today with the IXS method.

Ab initio calculation of the excitonic linewidth due to electron-phonon interaction in semiconductors

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In indirect band gap semiconductors at low impurity and carrier concentrations, the linewidth of the direct band gap exciton E_0 is controlled by the interaction of the excited electron with short-wavelength phonons [1-3]. This linewidth is temperature- and pressure-dependent, and is due to phonon-assisted scattering of the excited electrons from the Γ point to the local minima of the conduction band, which are lower in energy.

We report on *ab initio* calculation of the excitonic linewidth in GaP and in GaAs under pressure. LDA approximation was used to describe the topology of the conduction bands and the electronic wavefunctions in semiconductors. The phonon frequencies and the corresponding perturbations of the self-consistent potential were calculated in the framework of the Density-Functional Perturbation Theory. We have extended the calculation of the electron-phonon coupling for metals to the case of semiconductors: integration of the electron-phonon coupling over the final states has been performed with our TAU-ISDP extention of the *espresso* package [4].

Our results are in good agreement with experimental results of spectroellipsometry for both GaP and GaAs under pressure [1,2], thus giving confidence in the LDA description of the conduction band, which can be used for the prediction of properties related only to the conduction bands of semiconductors, such as electron-phonon interaction.

References:

[1] S. Zollner *et al.*, Phys. Rev. B **48**, 7915 (1993)
[2] A.R.Gõni *et al.*, Phys. Rev. B **41**, 10111 (1990)
[3] S. Guha *et al.*, Phys. Rev. B **48**, 7222 (1998)
[4] Quantum-Espresso Package: http://www.pwscf.org

Software integration and development within Nanoquanta

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Ch. Freysoldt(2), V. Olevano(2), Y. Pouillon(2)*, and M. Verstraete(2)

(1) Integration Team 9
(2) Nanoquanta / ETSF File Formats Team

IT9 is labelled as "the team for integration of theory and code development". Its task constitutes an important component of ETSF. Presently each node has complementary theoretical capabilities and software tools, that should be integrated (beyond some existing bilateral or multilateral exchange of data), after the period covered by the FP6 action. Regarding data files, the work is focused on the wavefunction files in a planewave basis, for which there is now one flexible and documented format [1], based on NetCDF [2]. For other file types (crystallographic data, pseudopotentials, etc.), the discussion and documentation of file formats and the development of interconversion utilities is ongoing.

The organisation of a mini-workshop in November 2005 has allowed further progress along these lines. In addition to the Nanoquanta / ETSF file format specifications, it is envisioned that, as a result of this mini-workshop, IT9 might make a request of funding of one or more computer scientists, paid by the network, whose task would be to write conversion utilities, or implement I/O routines in existing software, and later, create a package with all available Nanoquanta Free Software [3].

References:

[1] http://www.smartgroups.com/vault/nanoquanta_members/IT9-Coding-Files/SpecFFNQ_v1.1final.pdf
[2] http://www.unidata.ucar.edu/software/netcdf/
[3] http://www.smartgroups.com/vault/nanoquanta_members/IT9-Coding-Files/ReportMiniWkshpLLN_v4.pdf

Polarization Propagator Corrections to Linear Response Time-Dependent Density-Functional Theory for Molecules with Closed- and Open-Shell Ground States

M.E. Casida

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A decade ago time-dependent density-functional theory (TDDFT) was introduced to the quantum chemistry community in its linear response (LR) for calculating excitation spectra [1]. Since that time LR-TDDFT has become a method of choice for calculating molecular vertical excitation energies because of its demonstrated accuracy within the domain of applicability [2] determined by present-day approximate exchange-correlation functionals. One limitation of the method comes from the wide-spread use of the TDDFT adiabatic approximation which limits LR-TDDFT to quasiparticle spectra (i.e., one-electron excitations). Two-electron excitations are important when calculating the excitation energies of closed-shell molecules both (i) because of the importance in some molecules of excited states with substantial two-electron character and (ii) because the inclusion of two-electron excitations allows a better description of biradical ground states. Spin-flip excitations are a particular type of two-electron excitation which is important for a correct description of the excitation spectra of molecules with open-shell ground states. Some of these points are nicely illustrated in Ref. [3]. In this talk I plan to outline how the equation-of-motion superoperator approach may be used to derive nonadiabatic polarization propagator corrections [4] to adiabatic LR-TDDFT for application to the above mentionned problems.

References:

[1] M.E. Casida, in *Recent Advances in Density Functional Theory*, Vol. I, edited by D.P. Chong (World Scientic: Singapore, 1995), p. 155
[2] M.E. Casida, in *Accurate Description of Low-Lying Molecular States and Potential Energy Surfaces*, ACS Symposium Series 828, edited by M.R. Ho mann and K.G. Dyall (ACS Press: Washington, D.C., 2002), p. 199
[3] M.E. Casida, A. Ipatov, and F. Cordova, in *Time-Dependent Density-Functional Theory*, edited by M.A.L. Marques, C. Ullrich, F. Nogueira, A. Rubio, and E.K.U. Gross, Lecture Notes in Physics (Springer: Berlin, 2006)
[4] M.E. Casida, J. Chem. Phys. 122, 054111 (2005)

Is “Nano” that Different from the Bulk?

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(2) Central Michigan University, USA

Large-scale first principles computations for the optical absorption spectra of medium size Si clusters (with 20 to 28 atoms) are presented. The computations are performed using time-dependent density functional theory within the adiabatic local density approximation (TDLDA). We find that prolate and compact clusters have distinct shape signatures, but no clear size-dependence for a given shape in this size range. The shape dependence and size-independence of the spectra, and most of the peak positions and intensities can be explained remarkably well within the *classical* Mie theory, developed for light absorption by *metallic* particles, using the *bulk* dielectric function of Si. Moreover, the experimental spectrum of Si_{21} is in very good agreement with the theoretical spectrum of the prolate cluster, which is lower in energy than the compact one at this size. TDLDA results presented here for the dynamical response of Si clusters to time-varying electric fields provide further support for (i) their metallic behavior, as suggested in previous studies of their response to static electric fields and (ii) recent studies of static, but wavevector-dependent, screening in hydrogenated Si quantum dots, which have indicated that the bulk dielectric function is able to capture the essential screening in nano-objects as long as the appropriate boundary conditions are taken into account through classical electrostatics.

Electron-nuclear interaction from Time-Dependent Multi-component Density Functional Theory

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We use Time-Dependent Multi-component Density Functional Theory (TDMCDFT) to describe the electron-nuclear system fully quantum mechanically. In this theory the electron density and nuclear density matrix of the system are the fundamental variables. The approach allows to describe both the electron and the nuclear motion in the system.

We use TDMCDFT to treat electron-nuclear many-body effects, which are not described within the framework of pure electron Time-Dependent Density Functional Theory (TDDFT).

The success of the approach depends on the approximation for the exchange-correlation functionals used in TDMCDFT. The necessary exchange-correlation functionals can be derived on the basis of many-body perturbation theory.

Dielectric Function of Silicon for Finite Momentum Transfer – Signatures of Short-Range Many-Body Effects

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We present an investigation of the dynamic structure factor and of the dielectric function of the prototypical semiconductor silicon for finite momentum transfer, combining Inelastic X-Ray Scattering and ab initio calculations. We show that, in contrast to optical spectra, for finite momentum transfer Time-Dependent Density-Functional Theory in Adiabatic Local-Density Approximation together with lifetime broadening describes the physics of valence excitations correctly. Short-range crystal and exchange-correlation local-field effects become increasingly important with increasing momentum transfer. Major structures in the spectra are governed by a mixing of transitions of positive and negative energies, in striking difference to spectra for vanishing momentum transfer. This mixing gives rise to a pronounced Fano asymmetry in perfect agreement with experiment. Our results demonstrate the quantitative predictive power of the first-principles description.

Bethe-Salpeter equation from TDDFT perspective: Diagrammatic representation of the exchange-correlation kernel

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Many-body perturbation theory (MBPT) provides a regular method for the calculation of excitation spectra in interacting many-electron systems. Formal application of this approach reduces to the solution of Bethe-Salpeter equation (BSE) for a 4-point (or at least a 3-point) function, which is very demanding from the computational point of view. A promising alternative that has been intensively developed over last years relies on time-dependent density functional theory (TDDFT). The main advantage of this theory is that it requires the solution of a much simpler RPA-like equation with the Coulomb potential being replaced by an effective (and in general unknown) interaction, the exchange-correlation (XC) kernel. In this talk I establish an exact correspondence between MBPT and TDDFT. Starting from BSE, I show that the

corresponding ladder diagrams can be resumed to reduce the final theory to the TDDFT form. I derive an exact diagrammatic representation (and an integral equation) for the XC kernel, and discuss possible applications both for a construction of new approximations in TDDFT and for a development of new approximate schemes within MBPT.

Many-Body Perturbation Theory and Density-Functional approaches: successful combinations

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Today, in the framework of solid state physics two main ab initio approaches are used to describe ground- and excited state properties of condensed matter: on one side, static ground state density functional theory (DFT) and its time-dependent extension (TDDFT) for the description of excited states; on the other side, Many-Boby Perturbation Theory (MBPT), most often used in Hedin's GW approximation [1] for the electron self-energy, or the Bethe-Salpeter equation for the calculation of response functions.

Both approaches have led to breakthroughs, but suffer from different shortcomings: MBPT has a relative conceptual clarity and therefore allows one to find good approximations, but calculations are in general numerically very demanding. DFT-based approaches are in principle computationally more efficient, but a generally reliable and at the same time efficient description of exchange-correlation effects within TDDFT is difficult to obtain. In recent years several research groups (most of them within NANOQUANTA) have therefore worked on schemes to combine MBPT and TDDFT, searching for a formulation that would keep the advantages of both approaches.

Orbital-dependent linear response exchange-correlation kernels f_{xc} have been derived along different lines, including a mapping of the Bethe-Salpeter equation onto the TDDFT screening equation, a perturbative approach, diagrammatic expansions, a variational approach, or the use of the density-functional concept within Hedin's equations [2-6]. The different approaches have led to very similar results; in particular an approximation for f_{xc} was proposed that has been shown [2,3] to reproduce continuum and bound excitons for a wide range of materials.

This talk will give an overview of the various approaches, stressing their common content and discussing the success of the proposed approximations for f_{xc} as well as possible problems. The question of how to use such a combination in order to obtain vertex corrections to the self-energy will also be addressed [6].

As can be seen from the references, this talk represents contributions of a large number of colleagues.

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Control of electronic currents by laser in quantum rings

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We show that the excited states of N-electron semiconductor quantum rings (QRs) can be controlled by a circularly polarized laser field [1]. For this purpose, we define a realistic 2D model potential for the QR and treat the influence of a tunable laser field on the electrons with the dipole approximation. In the numerical calculations we apply the time-dependent density-functional theory within the OCTOPUS code package [2], which enables the evolution of the electronic wave functions in real time and real space. This allows us to monitor the total density and current in the QR during the propagation. As a generalization to a recent study on one-dimensional QRs [3], we find that (i) an external magnetic field creating persistent currents does not affect the controllability of the excited states, and (ii) the finite width of the QR considerably changes the dipole matrix elements required for the determination of the pulse length. Finally we discuss the prominent role of the electron-electron interactions as well as the possibilities to fully control the many-electron system by using the framework of the optimal control theory.

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Excitations in (bio)molecules from quantum Monte Carlo

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Despite significant progress in electronic structure methods, attaining an accurate description of the excited states of even relatively small organic molecules remains a demanding task. To this end, we have been developing a theoretical framework for the study of excited states based on quantum Monte Carlo methods. These correlated approaches are an alternative to conventional quantum chemistry and density functional methods, and have been successfully employed to accurately compute ground-state properties of large molecules and solid systems. Their application to excited states is however quite new and required a rethinking of some of the underlying concepts as well as further methodological developments. We will illustrate the performance of our approach with several photoactive (bio)molecules, and show a comparison with other existing theoretical first-principle methods considered promising for the computation of excited potential energy surfaces.

Work done in collaboration with F. Schautz, A. Scemama, M. Zaccheddu, and L. Guidoni.

Linear and non-linear dielectric response of periodic systems from quantum Monte Carlo

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We present a novel approach that allows to calculate the dielectric response of periodic systems in the quantum Monte Carlo formalism. We employ a many-body generalization for the electric enthalpy functional, where the coupling with the field is expressed via the Berry-phase formulation for the macroscopic polarization. A self-consistent local Hamiltonian then determines the ground-state wavefunction, allowing for accurate diffusion quantum Monte Carlo calculations

where the polarization s fixed point is estimated from the average on an iterative sequence. The polarization is sampled through forward-walking. This approach has been validated for the case of the polarizability of an isolated hydrogen atom, and then applied to a periodic system. We then calculate the linear susceptibility of molecular-hydrogen chains with different bond-length alternations. The results found are in excellent agreement with the best estimates obtained from the extrapolation of quantum-chemistry calculations. By adopting trial wavefunctions obtained from Hartree-Fock, we can then calculate with great accuracy the second hyper-susceptibility. Finally, we assess the importance of electronic correlations for the calculated linear and nonlinear susceptibilities.

Quantum kinetic simulations of electron transport in nanosystems

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In electronic devices of mesoscopic size the semiclassical Boltzmann kinetic equation is commonly used to calculate properties related to electron transport.

Boltzmann equation treats the electrons in terms of their classical probability distribution in phase space, and deals with collision events quantum-mechanically using Fermi golden rule. This formalism explains why conduction electrons subject to a uniform electric field do not accelerate indefinitely, but settle in a steady state regime of constant current, as a consequence of inelastic collisions with the lattice that lead to energy dissipation.

To describe transport in nanoscopic devices having spatial dimensions of the order of the electron wavelength, it is possible to generalize this method to the fully quantum mechanical case. Boltzmann equation is replaced by a quantum mechanical Liouville-master equation for a reduced density operator.

In this talk I present such a kinetic scheme based on a dissipative Liouville master equation. This approach can be used in the framework of a generalized time-dependent density functional theory for dissipative systems and can therefore be used for realistic nanoscopic systems.

In the presentation I will explain the formalism in detail and show its applicability in the case of transport through suspended carbon nanotubes.

An Approach to Quantum Transport Using TDDFT

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The Landauer formalism is a popular method to calculate the current through a nanoscopic system connected to two (or more) macroscopic electrodes and, in combination with techniques of density functional theory, is now widely used to compute current-voltage characteristics of single molecules. However, in the Landauer formalism the electrons are treated as non-interacting particles. In principle, the interaction can be included by Keldysh non-equilibrium Green's functions techniques but the resulting schemes are difficult to cast in a practical form. Time-dependent density functional theory offers a promising alternative description.

Here we present a description of transport based on the time evolution of the non-interacting time-dependent Schroedinger equation. We develop a numerical algorithm for the time propagation of extended states. For simple model systems, the scheme is used to compute the time-dependent current in response to an external dc or ac bias. As expected, for a dc bias the system evolves to the steady state predicted by the Landauer formula. The formalism is also used to study electron pumping in model systems. In the framework of time-dependent density functional theory the algorithm allows for the description of transport of interacting electrons beyond the Landauer formalism.

Non-equilibrium GW approach to electron transport in nanoscale contacts

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Correlation effects within the *GW* approximation have been incorporated into the Keldysh non-equilibrium electron transport formalism. We show that *GW* describes the Kondo effect and the zero-temperature transport of the Anderson model reasonably well. Combining the *GW* scheme with density functional theory and a Wannier function basis set, we illustrate the impact of correlations by computing the conductance of small molecules attached between metal leads. Our results indicate that self-consistency in the *GW* self-energy is fundamental for transport calculations.

Non-local self-energies in quantum transport calculations

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We calculate the conductance of a metal-vacuum-metal junction, where exchange-correlation effects are taking into account in terms of a gw-based non-local model self-energy operator. This conductance is then compared with the conductances predicted by both the local density approximated and exact Kohn-Sham theories built from the model self-energy. Significant deviations between these three conductances arise in the strong tunnelling regime. An attempt to connect these deviations with the band-gap problem of density functional theory is made. A brief discussion of the implementation of the self-energy model for atomistic models using a basis of localized numerical orbitals will also be given.

GW description of Correlation effects in Quantum transport on real systems

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In the framework of Non-Equilibrium Green's Function Theory (NEGF), we present an *ab initio* approach to electronic quantum transport in nanoscale systems which includes electron-electron interaction effects through a *GW* approximation on the Self-energy. With respect to DFT approaches to quantum transport, we use a real physical electronic quasiparticle structure into a Landauer-like expression for the conductance on a maximally localized Wannier functions basis. We take into account both the non-hermitean part of the *GW* Self-energy and also its full dynamical dependence, thus going beyond the plasmon-pole model. Preliminary results of a calculation on real systems, cupper and gold mono-atomic chains, will be shown. With respect to DFT, the *GW* conductance profile appears modified both by the hermitean part of the self-energy, which gives rise to a *GW* renormalization of the Kohn-Sham eigenvalues; and also by the non-hermitean part, which is associated to the finite lifetime of electronic states due to electron-electron scattering diffusion mechanisms and to the non coherent part of the electronic transport.

Dynamics of electrons and ab-initio modeling of quantum transport

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Within the many theoretical explorations addressing the steady-state ab-initio description of quantum transport there is relatively little material devoted to the problem of establishment of this steady state. The generally accepted points of view use the switching-on of the localised total electric field or the turning-on of the contacting between two initially biased electrodes. We argue that while both of these are equivalent none is satisfactory already at the time-dependent Hartree approximation. Instead, we show that employing an auxiliary homogeneous electric field turned on for a finite time does act as a source of current I which eventually leads to an induced drop in potential ΔV and thereby to the so called four-point conductance. We show how such a formulation is related to the character of the non-local dielectric function of the quantum junction.

Classical Nuclear Motion in Quantum Transport

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An *ab initio* quantum-classical mixed scheme for the time evolution of electrode-device-electrode systems is introduced to study nuclear dynamics in quantum transport. Two model systems are discussed to illustrate the method. Our results provide the first example of current-induced molecular desorption as obtained from a full time-dependent approach, and suggest the use of AC biases as a way to tailor electromigration. They also show the importance of non-adiabatic effects for ultrafast phenomena in nanodevices.

Kohn Sham gaps, potentials and excitation energies of finite systems using effective exact exchange-correlation potentials

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Conventional approximated exchange-correlation functionals are quite accurate in the prediction of total energy and ground-state conformation of different systems, but they yield quite poor Kohn-Sham(KS) spectra. The KS gap is too low or only works thanks to error compensation [1], and, in particular for finite systems, the highest occupied KS orbital eigenvalue much higher than the ionization potential and only few bound virtual orbitals are present. KS orbitals and eigenvalues are input quantities for time-dependent density functional theory(TD-DFT), thus they must be computed accurately in order to obtain accurate TD-DFT excitation energies. We show that the Localized Hartree Fock [2-4] method, an efficient effective exact exchange KS approach, can be extendend to include an ab-initio-like correlation potential. The non-local energy-dependent second-order self-energy operator [5,6] has been localized to obtain a local KS exchange-correlation potential. We propose a very efficient computational scheme and we present results for atoms, metal and semiconductor clusters, small and medium size molecules. Very accurate KS gap, KS potentials and TD-DFT excitation energies have been obtained.

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The effect of nonlocality on the band gap within density functional theory

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In this talk I compare the eigenvalue band gap found with a nonlocal potential within the generalized KS (GKS)[1] scheme and within the KS scheme using the optimized effective potential(OEP)[2] approach. Since I use the same exchange-correlation approximation (Coulomb-Hole screened-exchange) the difference in the band gap is due solely to the locality/nonlocality of the potential. In fact, I show that the difference between the OEP-KS and the GKS band gaps comes from the derivative discontinuity of the exchange-correlation energy that corresponds to the nonlocal potential [3].

Once the derivative discontinuity is taken into account, the corrected KS and generalized KS gaps are very close to each other. Finally I discuss whether the GKS schemes can be successfully applied to calculations of optical absorption spectra of semiconductors and insulators.

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Non-collinear magnetism within OEP with a view to spin dynamics

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The dynamics of spin degrees of freedom is responsible for phenomena like spin injection, spin wave excitations, spin filtering etc. These mechanisms are crucial for recent developments e.g. spintronics and spin transport. The advent of time dependent extension of SDFT has made the ab-initio treatment of spin dynamics possible. Crucial to the practical calculations using SDFT is the approximations made for the exchange-correlation energy functional. In calculations this is most often approximated with the LSDA, GGA or there time dependent extensions. These have been developed for collinear magnetism, and their use in non-collinear situations relies on the magnetisation ($\mathbf{m}(\mathbf{r})$) and exchange correlation magnetic field ($\mathbf{B}_{\mathrm{xc}}(\mathbf{r})$) being made collinear in a local reference frame at each point in space and at each time. Under such an approximation the $\mathbf{m}(\mathbf{r}) \times \mathbf{B}_{\mathrm{xc}}(\mathbf{r})$ vanishes everywhere in space. This renders all such calculations unsuitable for ab-initio spin dynamics in the adiabatic approximation, a serious limitation of the existing functionals.

In this conference I will talk about the generalization of OEP formalism for SDFT to non-collinear magnetic systems. Crucially, I do not rely on a condition of local collinearity. Using the exact exchange (EXX) functional and with the example of an unsupported Cr(111) monolayer, I will show that in general magnetisation and $\mathbf{B}_{\mathrm{xc}}$ are not parallel – in contrast to what is usually assumed in all to date non-collinear calculations. This renders the TD extensions of EXX functional suitable for the study of dynamical spin effects.

Additional many-body effects in the absorption spectra of Si nanocrystallites

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The quantum confinement of carriers in silicon nanocrystallites (NCs) gives rise to interesting properties such as the increase of the radiative recombination rates. The confinement properties of Si NCs have already been applied in electronic devices such as memories and may be useful for opto-electronic devices and detectors as well. Although an intensive experimental investigation on Si NCs has been carried out in the last two decades, the optical absorption and emission phenomena are not yet well understood. Since the results from experiments usually correspond to an ensemble of Si NCs with different sizes, theoretical investigations of a single Si NC become important to understand the mechanisms of light absorption and light emission in these nanoparticles. The traditional theoretical methods to calculate the absorption spectra based on density-functional theory and on the independent-particle Kohn-Sham scheme are very efficient nowadays, but they do not account for important many-body effects. We present ab initio investigation of Si NCs based on many-body perturbation theory for electronic excitation energies. The GW approximation (G stands for Green's function and W for the screened Coulomb potential) is used to calculate the quasiparticle energies and lifetimes. A dynamical screening is considered in the screened Coulomb potential W. The effects of the electron-hole interaction on the absorption spectra are investigated by means of a two-particle Hamiltonian combining the quasi-electron and the quasi-hole single particle states. We find that a redistribution of the states occurs in a wide energy range of the absorption spectra of Si NCs, which is qualitatively in agreement with results obtained within time-dependent density-functional theory (TD-DFT). The importance of each term in the two-particle Hamiltonian is discussed and compared with available results within TD-DFT.

Optical Spectra of doped Silicon Nanocrystals

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The absorption and the emission spectra of doped silicon nanocrystals including geometry optimization have been calculated within a first-principles framework. Starting from hydrogenated silicon nanocrystals, simultaneous n- and p-type doping with boron and phosphorous impurities have been considered. We found that the B-P co-doping results easier than simple B- or P-doping and that the two impurities tend to occupy nearest neighbours sites rather than other positions inside the nanorystal itself. The co-doped nanocrystals present band edge states localized on the impurities that are responsible of the red shifted absorption threshold with respect to that of pure un-doped nanocrystals in fair agreement with the experimental outcomes. The emission spectra show then a Stokes shift with respect to the absorption due to the structural relaxation after the creation of the electron-hole pair. Moreover the absorption and emission spectra have been calculated for a small co-doped nanocrystal by going beyond the single particle approach through the self-energy correction and the Bethe-Salpeter equation scheme showing the important role played by the many-body effects.

Exciton localisation of quasi one dimensional systems and optical properties

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Atomic chains and polymers are paradigmatic cases where it is known that TDDFT when used with local and gradient corrected density functionals does not give an adequate description of optical properties. We have performed calculations in Many Body Perturbation Theory including electron-hole interaction and in TDDFT using a new non local and energy-dependent kernel [1-3] for trans-polyacetylene and a molecular hydrogen chain. We show that this kernel that until now had been tested on bulk systems and surfaces gives very good results also for finite and quasi one dimensional systems when compared to Bethe-Salpeter results and experiments. The great overestimation of the ALDA in the calculation of the axial polarizability per monomer unit is partially corrected when the new kernel is used and we argue that the polarizability of long finite chains approach the infinte limit when the length of the chain reach the characteristic length of the size of the exciton of the infinite chain. Such localisation of the electron-hole wave function is due to the bond alternation of the polymer and dictates the saturation of the static polarizability with polymer length.

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Electronical and optical properties of the Si(113)-3×2 ADI surface: An ab initio study

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The electronical and optical properties of the high-index (113) surface of silicon with the 3x2 ADI reconstruction have been investigated using ab initio methods. The groundstate calculations for a periodic slab cell have been performed within the plane-wave pseudopotential approach to the density-functional theory as implemented in ABINIT. The optical properties have been obtained from the matrix elements of the momentum operator using the TOSCA package.

First of all, we have investigated the electronic density of states and, furthermore, the electronic band structure where we assigned the surface and the bulk states. These results are discussed in comparison with available experimental data.

The reflectance anisotropy spectra (RAS) has been calculated. A layer-by-layer analysis yields the surface contribution of the spectra, which has initially been derived for the full slab. The states which are responsable for the surface peaks have been identified. In the discussion, also available experimental and theoretical (tight-binding) reference data have been taken into account.

For all calculations, careful tests of the convergence parameters, e.g., the number of special points in the irreducible Brillouin zone, the slab thickness, the number of included conduction states, and the number of plane waves, have been performed.

Ab initio study of optical spectra for oxidized Si(100) surfaces

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Understanding the mechanisms of the oxide growth on the Si(100) surface is a key issue in the miniaturisation of the MOS devices. Research is prompted on the initial stages of the oxidation process as the gate insulators should be thinner than 2 nm [1]. Recently, surface-sensitive linear optical techniques like Reflectance Anisotropy (RAS) or Surface Differential Reflectivity (SDR) were applied for monitorizing in situ the Si(100) surface oxidation in its first stages [2]. However, the link between the way the surface is oxidized and its optical response is still not clear.

Using a plane-wave pseudopotential approach [3,4], we computed the RAS and SDR spectra for a set of representative surface models with nominal coverages from 0.5 ML to 1.5 ML (saturation for room temperature oxidation, molecular oxygen). Based on a model considering that at the surface many possible structures coexist, we were able to describe the evolution of both experimental RAS and SDR with exposure. For exposures up to 4.7 L, a model considering a mixture between two different oxidized surface models and a clean one can account for the changes in optical spectra starting from exposures as low as 0.6 L.

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Electronic Properties of Point Defects at the GaAs(110) and InP(110) Surfaces

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The electronic properties of semiconductor surfaces are strongly influenced by point defects that are either intrinsic or result from the accidental or intentional incorporation of impurities. Electrically active defects, in particular, may act as compensation centers and are responsible for Fermi-level pinning. Two important characteristics are the optical defect levels inside the band gap and the related charge-transition levels. The former can be probed by photoemission spectroscopy, for which the Franck-Condon principle is typically well justified, whereas the latter are thermodynamic quantities specifying the values of the Fermi energy where the charge state of the defect changes. As the theoretical results reported so far deviate significantly from experimental data, a quantitative determination of the electronic properties of individual point defects still remains a challenging task. The reason for the discrepancy lies in fundamental limitations of the computational schemes, which employed density-functional theory within the local-density approximation. As a remedy, we propose a new method that separates structural and electronic energy contributions and includes proper quasiparticle corrections. While the structural relaxation is well described by density-functional theory, we use the GW approximation for the self-energy in order to determine the electronic transition energies. In this way the discontinuity of the exchange-correlation potential as well as other shortcomings of commonly used functionals are treated appropriately. Our method is general and can be used to study point defects both at surfaces and in the bulk. As an example, we demonstrate its applicability for anion vacancies at the (110) surfaces of III-V semiconductors. For the P vacancy at InP(110) we find the (+/0) charge-transition level to be 0.82 eV above the surface valence-band maximum. Our result thus shows a clear improvement over the local-density approximation and is in very good agreement with the experimental value 0.75±0.1 eV. For the As vacancy at GaAs(110) we obtain 0.49 eV.

Propagation of the Kadanoff-Baym equations for many-electron systems

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We will present a general approach to solving the equations of motion of the nonequilibrium many-body Green's functions, commonly known as the Kadanoff-Baym equations. We implemented the time-propagation starting from a system in the ground state where for the self-energy we use the second order diagrams and the *GW* self-energy which are both conserving approximations.

In this way we can study the nonequilibrium properties of a wide variety of electronic systems such as atoms, molecules and quantum dots. The initial stage of the calculation requires solving the Dyson equation fully self-consistently for the equilibrium Green's functions. From these initial Green's functions we obtain total energies that we compare to results obtained from variational functionals of the Green's function. We also use time-propagation for calculation linear response functions as a means for obtaining the excitation energies of the system. In our scheme these response functions automatically satisfy important frequency sumrules.

Many-body and TDDFT methods for total energy calculations

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Since the pioneering works by Lein et al. [1] and Holm et al. [2,3]there has been an increasing interest in the evaluation of electron total energies using techniques either based on Many-body Perturbation Theory (MBPT) or on Time-dependent Density Functional Theory (TDDFT). These approaches are much more expensive than conventional implementations of the Kohn-Sham (KS) theory. However, they provide a truly first-principles description of electron-electron correlations without resorting to mean-field-like approximations, thus overcoming many well-known limitations of the KS-LDA or KS-GGA. On the other hand, these MBPT and TDDFT methods do not require the demanding computational effort of quantum Monte Carlo simulations and benefit from the continuous development of efficient algorithms to evaluate the relevant operators required to obtain both ground- and excited-state properties.

In the first part of this talk, I shall briefly summarize and compare both MBPT and TDDFT methods, focusing on their conceptual and technical advantages and limitations when applied to calculate electron total energies. In the second part, I shall concentrate on a recent application of TDDFT, where structural properties and vibrational spectra of hexagonal Boron Nitride are obtained [4]. This system is a paradigmatic example of layered material, where weak (dispersion-like) and strong (covalent) bonds coexist. The Kohn-Sham LDA and, specially, GGA badly fail when evaluating the layer-layer interactions. On the contrary, the in-plane and out-of-plane bonding is well described using TDDFT, also when the layers are pulled apart. This work paves the way for further implementations of truly ab-initio applications in systems where standard Kohn-Sham techniques lacks of predictive accuracy.

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An all-electron GW code based on FP-(L)APW+lo: the role of core electrons

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In recent years the *GW* approximation (GWA), typically applied as perturbation to DFT, has proven to be very successful describing quasi-particle excitations in semiconductors and insulators [1]. Most of the existing codes are based on the pseudopotential (PP) method, which is well established for ground state DFT calculations. In this scheme, the self energy is computed for the valence states only. There is, however, no guarantee that "core-valence partitioning" done in this fashion is also justified for the dynamical self energy, which is a highly non-linear functional of the total density. G_0W_0 results obtained with PP implementations are usually in better agreement with experiments than those reported from existing all-electron implementations. Self-consistent schemes allegedly improve the agreement of the all-electron calculations [2], but drastically worsen the PP results [3,4]. The reasons for this discrepancy and the necessity for self consistency are still a matter of debate [2,3].

In order to address these questions, we developed our own all-electron *GW* code. It is based on the FP-(L)APW+lo method, which currently provides the most reliable results within DFT. In this talk we will give a brief overview of the main characteristics of the code and show quasiparticle energy calculations for Si, GaAs and NaCl. By removing the core contribution to the self-energy and to the DFT-exchange correlation potential we analyze the validity of "core-valence partitioning" in *GW* calculations.

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Local and non-local vertex corrections in GW for extended and localised systems

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A non-local operator like the self-energy can be consistently calculated through many-body perturbation theory. This is usually done within the framework of the GW approximation which is obtained by ignoring vertex corrections in Hedin's equations. For a one-iteration G_0W_0 calculation it is only consistent to ignore the vertex correction if the starting point is the Hartree approximation. If the initial Green's function is obtained within a local approximation like DFT-LDA, there is in principle a local vertex given by the static exchange-correlation kernel in the first iteration [1]. We have implemented these local vertex corrections in Hedin's equations for jellium and closed-shell atoms. We present total energies and bandwidths for jellium and the equivalent quantities for He, Be and Ne. We show that a vertex implemented consistently in both the screened interaction and the self-energy leads to unphysical results and that an inclusion of the vertex in only the screened interaction provides results on par with or slightly better than standard G_0W_0. Finally, we discuss non-local vertex corrections derived from a non-local starting approximation for the self-energy and present preliminary results for jellium.

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First Principle Calculations of Band Offsets of SiO_2 and $ZrSiO_4$ with Silicon

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The size reduction of MOS transistor requires the usage of alternative materials to replace SiO_2 as gate oxide layers. The candidate materials so far were mainly high-κ oxides. As the high-κ/Si

interface is formed, it is crucial that the band offsets be large enough to prevent electron or hole injection. In this study first-principle DFT calculations within the local density approximation was used to estimate the band offsets of various interfaces, mainely, SiO_2 and $ZrSiO_4$ with Si. The many body corrections was included as calculated by *GW* approximation. The calculated band offets of SiO_2 were found to be in agreement with the existing experimental results.

The first-principle LMTO+U+SO+GW+T approach for the calculations of dynamic spin succeptibilities and life-times of excited electron in metals

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We develop a method for calculations of dynamic spin succeptibilities and life-times (inverse line-widths) of low-energy excited electrons in metals. The method includes the evaluation of the lowest term of self-energy within *GW* approach. The higher self-energy terms are also calculated within T-matrix approach. The T-matrix for the evaluations of the higher self-energy terms and spin succeptibility is obtained by solving Bethe-Salpeter equation with first-principle static RPA screened potential.

The method is based on the linear muffin-tin orbital (LMTO) approach for the band-structure calculations, including also U-corrections (LDA+U) and spin-orbital coupling (SO). The many-body calculations are performed in the basis of the products of LMTOs.

We discuss the results of the line-width and spin susceptibility calculations for Al, Au, Fe, Ni, Pd, Ta, Mo, Rh, Yb, comparing them with experimental data on photoemission spectroscopy, two-photon time-resolved photoemission spectroscopy, tunneling spectroscopy and experiments on measuring inelastic mean free path.

We find that the T-matrix terms of self-energy stronly depend on the details of the band-structure. For the metals with weak screening, i.e. Al, Au, Yb, they provide important contributions to self-energy, bringing the results of calculations in better agreement with experimental data.

We also discuss the ways of improving the methods of solving the Bethe-Salpiter equation in the LMTO basis set.

Posters

How to identify defects in carbon nanotubes : STM study and vibrational properties

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Scanning tunnelling microscopy (STM) and scanning tunnelling spectroscopy (STS) are powerful techniques for investigating the electronic topographic properties of nanomaterials. Whereas the already large amount of experimental STM data obtained so far on perfect nanotubes is perfectly understood, the identification of topological and non-topological modifications of the hexagonal lattice of a carbon nanotube remains an experimental challenge. Thanks to a simple, though accurate theoretical approach, it is possible to simulate the topographic and spectroscopic signatures of many types of defects in graphene and single-walled nanotubes, and to contribute therby to their identification from STM and STS observations. Several illustrations will be provided.

Effect of impurities on the optical properties of BN nanotubes

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The effect of impurities and defects on the optical properties of h-BN and BN nanotube were investigated using first-principle calculations. We showed that recent experiments of photoluminescence in BN nanotube can be explained by the presence of acceptor or donor levels in the band gap that occur in the visible and ultraviolet regions.

Identification of CdSe fullerene-based nanoparticles from optical spectroscopy calculations

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Semiconducting nanoparticles are the building blocks of optical nanodevices as their electronic states, and therefore light absorption and emission, can be controlled by modifying their size and shape. Likewise, optical properties can be a powerful tool to probe the atomic arrangement of synthesized nanoparticles. In view of that, we simulate light absorption of CdSe nanostructures with sizes up to 1.5 nm within density functional theory. We study both bulk fragments with wurtzite symmetry and novel fullerene-like core-cage structures. The comparison with experimental optical spectra allows to confirm the synthesis of these fullerene-based CdSe clusters.

A visualisation tool : V_Sim

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V_Sim [1] is a 3D visualisation program for atomic structures and spin representations. Several interactions are possible, such as, changing the view, displacing an atom, measuring distances and angles, or exporting into image files. Some advanced features allow to draw clipping planes, masking some portion of the rendered crystal ; or to colourise the atoms using some external data. Finally, several atomic files can be rendered one after another as if in a film while all interacting tools are still available.

The current development version includes some plug-ins capabilities allowing the creation of a reader for NETCDF files. Moreover the integration of the OpenBabel library, gives to V_Sim the capability to read a huge variety of file formats used both in the chemistry world and by physicists, such as CML, Gaussian output files...

This program is free software, using commonly used libraries such as OpenGL or GTK.

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Electronic excitations of oligoacenes in four different charge states: -1, 0, +1 and +2

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We present a systematic study of the electronic excitations for the five smallest oligoacenes (naphthalene, anthracene, tetracene, pentacene and hexacene) in their anionic, neutral, cationic and dicationic charge states. We used two different implementations of TDDFT. The low-lying electronic transitions computed by the two methods are found to be in good agreement with previous theoretical results and available experimental data. The strength of the excitonic effects has been also evaluated for the neutral systems. General trends in the electronic excitation properties are discussed as a function of the charge state and molecular size.

Optical properties of oxidized Si(100)(2x2) surface and local fields contributions on electron energy loss spectrum

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We use an efficient scheme to evaluate the independent particle dynamic polarization, used as a starting point in TDDFT to calculate the optical response of a system perturbed from a time dependent external potential. The method, based on an efficient use of the Hilbert transforms, has been implemented in a large-scale ab initio computational code, and the improvement of the scaling of the required CPU time with the system size has been carefully tested also checking the memory occupation of the algorithm and optimizing it. Previous results showing the application of this method to study the optical response of the oxidized Si(100)(2x2) surface on Reflectivity Anisotropy and Surface Differential Reflectivity spectra (RAS and SDR) motivated this work. The starting point of is the remark that the most important modification of the spectrum due to the local fields contributions comes from the component of the perturbing light with polarization perpendicular to the surface plane. We study here the optical response of the same system simulating the Electron Energy Loss Spectrum, where the response to the perpendicular component of the incident light, the most sensitive to the local fields effects, is involved.

Time-dependent electron localisation function: A tool to visualise and analyse ultrafast processes

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The time-dependent electron localisation function (TDELF) is a generalisation of the electron localisation function (ELF) proposed by A. D. Becke and K. E. Edgecombe [1], which allows for time-resolved observation of the formation, the modulation, and the breaking of chemical bonds, and can thus provide a visual understanding of complex reactions involving the dynamics of excited states. We discuss the rationale behind the definition of the ELF, and sketch the general derivation that permits its use for the analysis of time-dependent processes. We present some examples: First, ground-state results showing the characteristic topology of the ELF for various prototypical chemical cases. Secondly, the time-dependent ELF of a few processes is monitored, which demonstrates how it permits to enhance our visual intuition of the electronic behaviour during fast phenomena: the chemical reaction leading to the formation of the water molecule following the collision of a proton and a hydroxide ion, the capture of a proton by the lone pair of the electron rich, smallest imine or unprotonated Schiff base (formaldimine), and the bond breaking of the ethyne triple bond due to the interaction with a strong and ultrashort laser pulse.

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Study of the small-q contribution to the polarizability and the intraband term: from the jellium to the periodic solid

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The computation of the *GW* correction for a bulk jellium shows the importance of considering the intraband contribution in the q→0 limit for the polarizability since its absence induce the appearance of a gap. To include this contribution to the polarizability we propose an approach that avoids the Fermi surface integration, which would require a heavy numerical cost. The approach we propose is based on the idea of detrmining the limiting behaviour of the polarizability

by a fit of its Taylor expansion in the finite small-q region, where the standard computational approach has no numerical problems in evaluating the intraband contribution. In this way we expect will to be able to perform computations not only for the jellium, case in which the RPA polarizability is analitically known (the Lindhard function), but also for real solids.

Our work starts from bulk jellium since the system is simpler, the off-diagonal terms of the polarizability matrix are identically zero, and the polarizability depends only by the modulus of the wave-vector. In this case we know the limiting behavior for the different frequencies. The next step has been to traspose what we learned by the study of the jellium model on the general case. In this situation we deduced the limiting behaviour by theoretical consideration and by the comparison with test simulations.

Thiol adsorption effects on Au(111) work function

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The interface between SAMs and gold surfaces, in particular the Au(111), is one of the most investigated hybrid systems [1-4]. A lot of information is available about the conformation of the adsorbate and the energetic properties of methanthiol on Au(111)[2]. Due to the large computational costs required for these systems, usually short-chain thiol molecules have been investigated ab initio. In particular, being the S-metal interaction dominant in the molecular adsorption geometry, the attention has focused on methanthiol on Au(111), treated as a prototype for SAMs-metal interface. Among electronic properties of these systems, it is known that short chain alkanethiols adsorbed on gold induce a work function reduction [5]. Reported values for Au work function range from 5.0 to 5.3 eV [1,6], and the thiol induced reduction is of 1.2 eV, with maximum values of 1.4 eV [7].

Here, we investigate the effect on the gold work function of adsorbed methanthiol and of CH3(CH2)5SH (hexanethiol) which introduces the effect of the long alkyl chain on the workfunction. Ab initio calculations have been performed in the framework of DFT, using the plane-waves code PWSCF [8], the PW91 parameterization [9] for the exchange-correlation potential, and UltraSoft Pseudopotentials [10]. The coverage of 1 ML corresponds to one thiol molecule for three Au surface atoms, in the hexagonal adsorption geometry. Different adsorption sites and coverages have been calculated to understand the work function behaviour, obtaining results in good agreement with experimental findings.

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All-Electron GW Approximation in the Augmented-Plane-Wave Basis-Set Limit

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The GW approximation for the electronic self-energy is known to yield quasiparticle band structures in much better agreement with experimental measurements than the local-density approximation (LDA) for a large class of materials. However, almost all actual implementations so far are based on the plane-wave pseudopotential approach, which effectively restricts applications to simple metals and sp-bonded semiconductors. In order to overcome this limitation, we have developed an alternative implementation within the all-electron full-potential linearised augmented-plane-wave (FLAPW) method, which is also applicable to systems with localised electrons like transition metals or rare-earth elements. Additional simplifications, such as plasmon-pole models, are avoided.

While the FLAPW method treats the core electrons explicitly and does not suffer from the uncontrolled pseudisation of the wave functions, another source of errors resulting from the linearisation is frequently overlooked. It arises because the radial wave functions in the muffin-tin spheres are expanded around fixed reference energies. Irrelevant for the valence bands in density-functional theory, it cannot be ignored in the *GW* approximation, where unoccupied states more than 100 eV above the Fermi level must typically be included in the self-energy to guarantee converged results. To eliminate this error, we have extended the FLAPW basis set by including second and higher energy derivatives of solutions to the radial scalar-relativistic Dirac equation in the form of local orbitals. With this modification, we show that the linearisation error is eliminated and the basis set becomes complete. In the case of spherical muffin-tin potentials the results in the basis-set limit are identical to augmented-plane-wave calculations. This careful approach finally allows us to comment on the controversy surrounding the apparant discrepancy between pseudopotential and all-electron *GW* results addressed in several recent studies [1,2]. For the example of silicon, we demonstrate that the inclusion of a much larger number of unoccupied states and the elimination of the linearisation error both contribute to an increase of the band gap. While a certain deviation from pseudopotential calculations remains, it is smaller than previously claimed, and both results lie in comparable proximity to the experimental value.

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Single-particle excitation energies starting from generalized Kohn-Sham schemes

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The *GW* approximation of Hedin is arguably the most successful approach for the calculation of quasi-particle (QP) energies. Its accuracy has been proven for a variety of systems. Usually, the QP eigenvalues are calculated in a perturbative approach, starting from solutions of the Kohn-Sham equations with an exchange-correlation (XC) potential in local density or generalized gradient approximation (LDA/GGA). However, this standard approach fails for a number of systems such as InN which share shallow semi-core electrons and a negative gap in LDA/GGA. Here we present *GW* calculations for Si, ZnO and InN which start from solutions of the generalized Kohn-Sham (gKS) equations [1] for the screened exchange (sX [1]), HSE03 [2], PBE0 [3] and HF model of exchange and correlation. Such a procedure is found to yield a positive gap for all the investigated gKS functionals. Furthermore, with exception of HF the resulting gaps are almost the same for all the gKS functionals choosen as starting point. The results are critically analysed with respect to the wave-function character and localization. In addition we discuss the influence of different core-valence XC models. The calculations were performed using a model dielectric function for the *GW* self-energy. The electron-ion interaction was modeled via the PAW method which provides direct access to the all-electron wave functions.

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Excited states of formamide in water

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The electronic structure of liquid water is still not fully elucidated, even though it is essential to understand the chemical and physical properties of many biochemical and industrial processes that occur in solution, where it is crucial to include the role of the solvent in the reactions.

Excited state properties have not been investigated yet, neither for pure water, nor for water as a solvent. We present here ab-initio calculations of pure liquid water and of a solution of formamide. We use snapshots taken from molecular dynamics as input geometries for the study of the electronic and optical spectra. The optical absorption spectra are first obtained within the Density Functional Theory and then calculated by solving the Bethe-Salpeter equation. We show that the effect of the solvent on the optical spectra of the solution can not be neglected.

Nonlocality and frequency dependence of effective potentials

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Many-body perturbation theory (MBPT) [1] is a very powerful method. The key variable is the Green's function $G(r, r', \omega)$ which contains a great deal of information, like the one-quasiparticle spectra. However, one is often interested in just a part of the information carried by G, so in these cases it is preferable to work with simpler quantities from the beginning. This is precisely the case of density-functional theory (DFT) [2], where one wants to obtain the ground-state total energy and density $\rho(r)$. In principle, one doesn't need the full G to obtain this information. In the Kohn-Sham approach [3] it is sufficient to solve an effective one-particle Schrödinger equation, with a local and static potential $V_{xc}(r)$. The Green's function, in turn, is determined by a nonlocal and frequency dependent self-energy $\Sigma(r, r', \omega)$. A possible link between DFT and

MBPT is the Sham-Schlüter equation [4]:

$$V_{xc}(r_1) = \int d\omega dr_2 dr_3 dr_4 \times$$

$$e^{i\eta\omega}\,\tilde{\chi}^{-1}(r_1,r_4)G_{KS}(r_4,r_2,\omega)\Sigma(r_2,r_3,\omega)G(r_3,r_4,\omega)$$

$$\tilde{\chi}(r_1,r_2) = \int d\omega\, e^{i\eta\omega} G_{KS}(r_1,r_2,\omega)G(r_2,r_1,\omega)$$

Here we generalize the Sham-Schlüter equation to situations where one is interested in other parts of the Green's function. For example, one can consider the trace of the spectral function, which is needed to interpret photoemission spectra. In this case a local and dynamical potential $V_{SF}(r,\omega)$ can be introduced. We show that in this case the nonlocality of the self-energy can be converted into a frequency dependence of V_{SF}. This is illustrated for model systems. We discuss also the link with dynamical mean-field theory (DMFT) [5] and other approaches.

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Electronic excitations in Vanadium Oxide (VO$_2$)

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Vanadium Oxide has a metal-insulator transition at $T_C = 340$ K. The role of correlation in this first-order transition has been debated for a long time (see, for instance, Ref. [1,2]): is VO$_2$ a Peierls or a Mott-Hubbard insulator?

Despite a good agreement with experimental lattice parameters, DFT-LDA yields a negative gap in the insulating phase and hence is not able to give a good answer to this question. This seeming failure of LDA is discussed and different possible approaches to solve this problem are reviewed: from standard perturbative G_0W_0 to self-consistent *GW* [3,4]. Also results concerning other kinds of electronic excitations (in particular: electron energy loss spectra) are presented.

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Ab Initio calculations of graphene like systems

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We study the possibility to simulate with planar systems, optical absorption and EEL spectra of graphite nanotubes. The calculations are performed ab initio using TDDFT method. We calculate the electronic excitations of graphite and graphene like systems. More specifically, we study the influence of the distance between planes, as well as their stacking to characterize interaction between tubes and walls in multi-wall nanotubes. We also develop a simple model to calculate systems with large inter-plane distance using as reference the system with a smaller one, in order to reduced the size of calculations. The band structure calculations are done using Abinit [1]. The spectra are calculated using DP [2].

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Anisotropy in EEL-spectra for large momentum transfer

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Using Time-Dependent Density Functional Theory (TDDFT), we studied Electron Energy Loss Spectra (EELS) for different graphitic systems at large momentum transfers q. In particular, we investigated their anisotropy with small deviations in q, which seems to occur not only for vanishing (q=0), but also for large momentum transfer, corresponding to reciprocal lattice vectors (q=G) and should be attributed to local-field effects (LFE).

Finite Element Implementation of Green's Function Method for Transport Problems in Nanostructures

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A popular method to model electron transport in nanostructures is to use the simple ballistic transport model including interactions within the density functional theory. We have applied the scheme using the Green's function method which avoids the calculation of electron wavefunctions. Thereby a nanostructure can be connected to the leads by open boundary conditions. Within the nonequilibrium formulation it is also possible to add a finite bias voltage between the leads and calculate the current in a non-linear fashion.

We have implemented the scheme using the finite element method with the so-called p-elements for one-, two- and three- dimensional problems in order to model several types of nanostructures. The method allows a systematic error control and it is not restricted to a particular type of a problem. Moreover, the use of higher order elements results in a convergence which is faster than that obtained by the finite difference method. For the electron-ion interactions we use non-local norm-conserving pseudopotential operators.

We have applied our implementation to model the insulating properties of thin HfO2 layers, two dimensional quantum point contacts, and a magnetic resonant tunneling diode.

Towards a reduced density matrix functional theory for solids

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Reduced-density-matrix-functional theory (RDMFT) is one possible way to treat electron correlation beyond density-functional theory. In order to calculate the fundamental gap we generalize RDMFT to fractional particle numbers. For each fixed particle number, M, the total energy is minimized with respect to the natural orbitals and their occupation numbers. This leads to a function, E_{tot}^{M}, whose derivative with respect to the particle number has a discontinuity identical to the gap. Numerical results are presented for alkali atoms, small molecules, and periodic systems.

Within RDMFT the correlation energy is approximated in terms of the one-body reduced density matrix. One drawback of the first generation functionals is their failure to reproduce the correlation energy of the spin-unpolarized homogeneous electron gas (HEG). Recently, new functionals were introduced which considerably improve the results for atoms and molecules [1]. We apply these functionals to the HEG and show that they also improve the results dramatically. Furthermore, we generalize the second-generation functionals in such a way that they reproduce the correlation energy of the HEG exactly over the whole range of electron densities. We discuss ways to apply the resulting functionals to both finite and inhomogeneous periodic systems.

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Optical properties of the Sb-stabilized GaSb(001) surface

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Thin film InAs/GaSb semiconductor heterostructures show great promise as components of micro- and optoelectronic devices. A proper understanding of the interface formation requires,

however, a thorough understanding of the (clean) GaSb surface before adatom deposition. In spite of several experimental studies of the surface [1], few realistic calculations exist. The structure remains a matter of some controversy, with several c(2x6) and (4x3) reconstructions being proposed on the basis of total energy calculations [2]. The surface sensitivity of reflectance anisotropy (RA) spectroscopy makes it possible to identify (by means of a combined experimental and theoretical approach) the correct surface structure and to understand the underlying electronic structure. High quality experimental data is indeed available for this surface [3]. Of particular interest is the role of heterodimers, which have recently been shown to characterize the RA spectra of GaAs [4]. Recent tight-binding calculations [5] have shown that spin-orbit effects can have considerable and unpredictable effects on RA spectra for compounds containing antimony (Sb). In bulk GaSb, the hole spin-orbit splitting at the Brillouin zone centre is almost as large as the direct gap itself (about 0.8 eV). Hence we also investigate the influence of spin-orbit coupling on the optical properties, using a specially developed interface between the quantum-espresso and SELF codes [6].

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Vertex corrections in localised and extended systems

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Many-body perturbation theory (MBPT) is a leading method for excited-state calculations. It has also been shown to yield good results for total energies. Within MBPT, GW is the most widely used approximation to the self-energy. This ignores the vertex function, setting it to unity. However this is only theoretically justified if the non-interacting Green's function used initially is made from Hartree wavefunctions. This is a poor starting point and in practice we use Density-Functional Theory (DFT) wavefunctions: there is no theoretical justification for this though.

We use the methods of Del Sole *et al.* [1] which we call GW-LDA and $GW\Gamma$-LDA.These use the static exchange-correlation kernel, Kxc, in the vertex function to correct for the DFT starting point. We apply these methods to atomic systems and compare to GW-RPA.

We show that GW-LDA gives similar results to GW-RPA for total energies and first-ionisation energies. However $GW\Gamma$-LDA is poor compared to GW-RPA. We also present results for bulk systems showing that GW-LDA gives more accurate bandwidths than GW-RPA and $GW\Gamma$LDA and compare to a simple non-local vertex.

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Photoexcitation of Disperse Red 1: Comparison of Approaches

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Disperse Red 1 (DR1) is a 38 atomic azobenzene molecule with nonlinear optical response due to its delocalized electrons [1]. We test several one-electron methods, including Hartree-Fock and selected Density Functional Theory (DFT) approximations for prediction of the molecular structure and related photoexcitation within the dipole approximation. Also exact exchange (EXX), and Time-Dependent DFT (TDDFT) approaches [2] are considered [1,3-5].

In one-electron picture the HOMO-LUMO transition is forbidden due symmetry, emphasizing the role of transition probabilities. The TDDFT results do not essentially depend on the chosen exchange-correlation functional and turn out compare best with experimental absorption spectra [1,6]. Performance of the other approaches is discussed.

Success of the rapidly evolving real-space methods is also considered.

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LDA+DMFT computation of the electronic spectrum of NiO

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The electronic spectrum, energy gap and local magnetic moment of paramagnetic NiO are computed by LDA+DMFT(QMC). To this end the noninteracting Hamiltonian obtained within the local density approximation (LDA) is expressed in Wannier functions basis, with only the five anti-bonding bands with mainly Ni 3d character taken into account. Complementing it by local Coulomb interactions one arrives at a material-specific many-body Hamiltonian which is solved by dynamical-mean field theory (DMFT) together with quantum Monte-Carlo (QMC) simulations. The large insulating gap in NiO is found to be a result of the strong electronic correlations in the paramagnetic state. Although the energy gap calculated in this way is of Mott-Hubbard rather than charge-transfer type, the shape of the electronic spectrum in the vicinity of the gap region is in good agreement with the experimental x-ray-photoemission and bremsstrahlung-isochromat-spectroscopy results of Sawatzky and Allen. The value of the local magnetic moment computed in the paramagnetic phase (PM) agrees well with that measured in the antiferromagnetic (AFM) phase. Our results for the electronic spectrum and the local magnetic moment in the PM phase are in accord with the experimental finding that AFM long-range order has no significant influence on the electronic structure of NiO.

Modifications of BSE Due to Spin Polarization: Antiferromagnetic MnO

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Extensive studies of optical properties beyond the independent-particle approximation using the Bethe-Salpeter equation (BSE) have been performed for a wide range of materials, such as bulk semiconductors, surfaces, and molecules. As spin-polarized systems gain more and more interest, it is desirable to describe also their excitation properties within this approach.

Therefore, we consider the effect of spin polarization on the optical properties of materials with collinear magnetization. The Bethe-Salpeter equation for such systems starting from a *GW* treatment of the electronic self-energy contribution is derived. An electron-hole exchange term is taken into account in order to describe local-field effects in the macroscopic dielectric function.

We present numerical results for the antiferromagnetic insulator MnO which can be treated as a paradigmatic example for such a spin-polarized system. The one-particle wave functions are calculated in density-functional theory (DFT) within the generalized-gradient approximation (GGA) using the projector-augmented wave (PAW) method. The screening of the Coulomb interaction in the effective two-particle Hamiltonian is described by a model dielectric function. Instead of solving the eigenvalue problem of the Hamiltonian, an equivalent initial-value problem is considered.

Magnetic phase diagram of the Mn-based Heusler alloys from first-principles

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The magnetic phase diagram of the Mn-based semi- and full-Heusler alloys are determined at T=0 using first-principles calculations in conjunction with the frozen-magnon approximation. We show that magnetism in these systems strongly depends on the number of conduction electrons, their spin polarization and the position of the unoccupied Mn 3d states with respect to Fermi energy. Various magnetic phases are obtained depending on these characteristics. Conditions leading to diverse magnetic behavior are identified. We find that in the case of large conduction electron spin polarization and unoccupied Mn 3d states far from the Fermi level an RKKY-like ferromagnetic interaction is dominating while antiferromagnetic superexchange becomes important in the presence of large peaks of unoccupied Mn 3d states close to the Fermi energy. The overall magnetic behavior depends on the competition of these two mechanisms. The obtained results are in very good agreement with the available experimental data.

Second order harmonic generation in crystalline semiconductors

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A comprehensive understanding of the nonlinear optical properties of solids is crucial for the improvement of nonlinear materials and devices and provides an opportunity to search for new materials. However, the theoretical description of nonlinear effects in solids is a formidable task and important difficulties have delayed any accurate calculations for many years.

We formulate a derivation for the calculation of second-order susceptibility tensor for crystals of any symmetry [1]. For cubic symmetries, we show how this approach can be simplified and expressed in terms of the second-order density response function and of the dielectric function. Numerical results will be presented for SiC and GaAs.

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Entanglement in Anderson Nanoclusters

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We investigate the two-particle spin entanglement in magnetic nanoclusters described by the periodic Anderson model. An entanglement phase diagram is obtained, displaying the role of the entanglement in the temperature dependent competition between local Kondo screening and nonlocal Ruderman-Kittel-Kasuya-Yoshida spin ordering. This provides an entanglement perspective on a central property of magnetic nanoclusters. We also show that multiparticle entangled states are present for finite magnetic field as well as in the mixed valence regime and away from half filling.

Magnetic field effects on optical and transport properties in InAs/GaAs quantum dots

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A photoluminescence study of self-assembled InAs/GaAs quantum dots and under influence of a magnetic field perpendicular to the dot layer is presented. At low temperatures, the magnetic field alters the in-plane transport properties due to localization of carriers in WL potential fluctuations. Decreased transport in the WL results in a reduced capture into the quantum dots and consequently a weakened dot related emission. The effect of the magnetic field exhibits a

considerable dot density dependence, which confirms the correlation to the in-plane transport properties. An interesting effect is observed at temperatures above approximately 100K, for which the magnetic field induced an increment of the quantum dot photoluminescence. This effect is ascribed to the magnetic confinement of the exciton wave function, which increases the probability for carrier capture and localization in the dot.

The GW space-time formalism at finite temperatures

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We present the generalization of the space-time formulation of the *GW* approximation in many-body perturbation theory. The main changes are introduced in the treatment of the imaginary time and frequency dependency of the polarizability, screening, and self-energy. The discrete Matsubara frequencies and finite imaginary time intervals for integration are taken into account. Efficient fitting and interpolation schemes are developed to avoid a large increase in the grid sizes when going to metallic and finite-T systems.

Electronic excitations in hexagonal layered systems (C and BN)

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We present different phenomena involving electronic excitations in layered systems. For hexagonal boron nitride (BN), we show that excitonic effects play an important role for the optical properties. Measured and calculated values for the band-gap still display a strong scattering between 4.3 and 6.8 eV. We show that optical absorption and electron energy loss spectroscopy

cannot be explained in terms of independent-electron transitions but can be properly understood only by proper inclusion of excitonic effects. We discuss the origin of the different values for the measured/calculated band-gaps. For the interpretation of Raman spectra of graphite, the double-resonant Raman model which involves electron-hole pair excitations is qualitatively successful. Quantitative evaluation based on DFT band-structures display, however, a mismatch between theory and experiments. We discuss the achievements and short-comings of the double-resonant model for the explanation of the differences in the Raman spectra of single-layer, few-layer, and bulk graphite.

Ab initio calculation of structural and electronic properties of InAs and GaAs having wurtzite crystal structure

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The growth of new materials is a frequently occurring event in current semiconductor physics. The novelty of the fabricated systems demands a theoretical study of their structural and electronic properties which will provide the necessary knowledge to exploit their features, corroborate the experimental analysis and design the materials of the future.

Motivated by the finding that InAs NanoWires (NWs) grow purely wurtzite and GaAs NWs as a mixture of zinc-blende and wurtzite crystal structures, we focused our attention on the study of the latter polymorph for which no previous calculations exist.

We report our results on ab initio calculations of bulk InAs and GaAs having wurtzite structure. All-electron plane wave calculations within the DFT/LDA approximation are used to obtain the structural properties and the electronic band structure. The latter is computed with and without the inclusion of the Spin-Orbit interaction. The role played by the d electrons is investigated with the use of pseudo-potential calculations.

To properly describe the excited-state properties a method based on many-body perturbation theory is needed. Hence, the quasiparticle band structure was calculated whithin the GW approximation for both materials and for both polymorphs, finding good agreement with very recent experimental results.

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