

**0.1 Report on the 12th Nanoquanta Workshop on Electronic Excitations.
Time-Dependent Density-Functional Theory: Advances and Prospects**

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The workshop gathered 120 participants from leading international theory groups. There were 46 oral presentations (23 invited speakers and 23 contributed talks) and 32 posters. The workshop allowed the participants to discuss the advances in the theoretical and computational treatment of optical and dielectric spectroscopy, photoemission spectroscopy and quantum transport in the framework of time-dependent density-functional theory (TDDFT), many-body perturbation theory (MBPT) and non-equilibrium Green's function (NEGF) theory.

Invited speakers from leading international groups gave an in-depth overview of current research activities within these theories 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 advances and perspectives in time-dependent density-functional theory. Indeed, the first session presented two review talks on TDDFT and DFT-like methods applied to quantum transport. A particular effort has been done by the two invited speakers to present the arguments in the most pedagogical manner, *ad usum* of the youngest participants to the workshop. The next session rather focused to new methodologies implemented into TDDFT. Two sessions (Wednesday 19 afternoon) presented applications of TDDFT to complex technologically important systems and discussed also the relevance of commonly used approximations to TDDFT, as well as advances with respect to these approximations. There was also a session presenting advances in TDDFT theory coming from conserving approximations in MBPT and NEGF (Friday 21 late morning).

A session (Tuesday 18 afternoon) was devoted to core-electron spectroscopy and in the same session a speaker was invited to present advances obtained into one of the most recent experimental technique, the Resonant Inelastic X-ray Spectroscopy (RIXS), which is going to have in the next years an important role in driving advances within theory.

A series of two sessions (Wednesday 19 morning) were completely devoted to quantum transport, 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. The analyzed applications ranged from models to nanostructures, up to biological systems.

A session (Thursday 20 morning) was devoted to DFT or density-matrix functional theory approaches toward an exact treatment of the exchange and correlation, while the next one treated carbon based systems, both addressing quantum transport properties and also optical and Raman spectroscopy.

The GW method has, as usual, received much attention by this meeting. Both self-consistency, all-electron vs pseudopotentials and beyond GW issues were treated, as well as new implementations into localized basis set. Implementations of spin degrees of freedom (Friday 21 morning) and spin-orbit coupling into the Bethe-Salpeter equation and more in general many-body methods, as well as other interesting effects like those due to the electron-phonon (leading up to superconductivity) and the electron-magnon interaction have been presented here and there along the conference.

Finally, several presentations have indicated the strongly correlated systems as a new and interesting domain for *ab initio* excited state theories. Both advances of the theory and new successful calculations on strongly correlated systems were presented.

Very interesting discussions took place on the complementarity of the two methods, TDDFT and NEGF, toward a description of quantum transport properties.

It is worth to notice that the state-of-the-art implementations of all the above mentioned *ab initio* methods into existing numerical codes was presented in this meeting.

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 (some are still missing) and are going to be 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.

0.1.1 Programme

| Monday 17 | |
|-----------|----------------------------------|
| | |
| 16:00 | Registration |
| 17:00 | Nanoquanta Steering Committee |
| 20:00 | Welcome Dinner |

| Tuesday 18 | |
|------------|------------------|
| 09:00 | Welcome |
| 09:05 | Gross |
| 09:50 | Burke |
| 10:20 | Coffee Break |
| 10:50 | Marques |
| 11:20 | Castro |
| 11:40 | Pouillon |
| 12:00 | Lunch |
| 14:30 | Palummo |
| 15:00 | Freysoldt |
| 15:30 | Rohlfing |
| 15:50 | Coffee Break |
| 16:20 | Braicovich |
| 16:50 | Soininen |
| 17:20 | Fratesi |
| 17:40 | Poster Session + |
| 18:30 | Aperitif |
| 20:00 | Dinner |

| Wednesday 19 | |
|--------------|-------------------------------|
| 09:00 | Pantelides |
| 09:45 | Hannewald |
| 10:15 | Coffee Break |
| 10:45 | Mostofi |
| 11:15 | Ness |
| 11:35 | Verstraete |
| 11:55 | Lunch |
| 14:30 | Côté |
| 15:00 | Maitra |
| 15:30 | Coffee Break |
| 16:10 | Chelikowski |
| 16:40 | Grüning |
| 17:00 | Nanoquanta General Meeting |
| 20:00 | Gala Dinner |
| 21:30 | I3 ETSF Party |

| Thursday 20 | |
|-------------|----------------------------------|
| 09:00 | Scheffler |
| 09:30 | Helbig |
| 09:50 | Bokes |
| 10:10 | Coffee Break |
| 10:40 | Lazzeri |
| 11:10 | Zanolli |
| 11:40 | Varsano |
| 12:00 | Lunch |
| 14:30 | Pasturel |
| 15:00 | Blase |
| 15:30 | Coffee Break |
| 16:00 | Li |
| 16:20 | Gierlich |
| 16:40 | Nanoquanta IT1, IT9 Meetings |
| 20:00 | Dinner |
| 21:30 | Nanoquanta Steering Committee |

| Friday 21 | |
|-----------|--|
| 09:00 | Rödl |
| 09:30 | De Fausti |
| 09:50 | Schleife |
| 10:10 | Coffee Break |
| 10:40 | Hellgren |
| 11:10 | van Leeuwen |
| 11:40 | Stan |
| 12:00 | Lunch |
| 14:30 | Bockstedte |
| 15:00 | Marini |
| 15:20 | Ren |
| 15:40 | Coffee Break |
| 16:10 | Ferretti |
| 16:30 | Sasioglu |
| 16:50 | Nanoquanta Young Reaserchers Meeting |
| 20:00 | Dinner |

| Saturday 22 | |
|-------------|-------------------------|
| 09:00 | Gatti |
| 09:30 | Martin-Samos |
| 09:50 | Luppi |
| 10:10 | Coffee Break |
| 10:40 | Andrade |
| 11:00 | Abedi |
| 11:20 | Farewell |
| 12:00 | Lunch |
| 13:15 | Departures |
| 14:30 | Nanoquanta EU Review |

0.1.2 Oral Presentations

Limitations of present DFT calculations of transport

Kieron Burke

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Abstract

I will discuss several distinct reasons for why present DFT calculations of transport, which combine ground-state DFT and the Landauer formula, might be highly inaccurate.

(1) Even within the standard approach, common approximate functionals do not include a derivative discontinuity or correct for self-interaction. This can both misalign levels and broaden resonance peaks when a molecule is weakly coupled to leads.

(2) In the weak bias limit, one can use Kubo linear response theory to deduce the exact conductance. We find the Landauer formula misses XC field effects, which likely reduce the conductance.

(3) For finite bias, several alternative schemes are being constructed that may or may not reduce to the Landauer formula (with XC corrections).

All references can be found in the review:

arXiv:cond-mat/0703591 (<http://chem.ps.uci.edu/~kieron/dft/>)

The frequency dependent Sternheimer equation in TDDFT

Miguel A. L. Marques

Centre for Computational Physics, Department of Physics, University of Coimbra

Abstract

Often we are interested in the response of an electronic system to a weak perturbing field. These underlie many different spectroscopy tools, and are therefore a window to the quantum mechanical world. It is then of little surprise that a multitude of methods appeared over the years to calculate response properties. In this talk, we look at a very old method: the solution of the Sternheimer equation. It is well known that this is the method of choice when calculating static response, like static polarizabilities, phonon frequencies, etc. Although a perturbative technique, it avoids the use of empty states, has a quite good scaling (N^2) with the number of atoms, and a relatively small prefactor.

The Sternheimer method can be trivially extended to frequency dependent perturbations, giving us access to a variety of dynamic responses. The simplest of these is perhaps the dynamic polarizability α . With basically the same effort we can access the first hyperpolarizability β , that is responsible for the processes of second-harmonic generation, optical rectification and Pockles effect. Van der Waals C_6 coefficients are obtained by changing the frequency of the perturbing field from real to imaginary. Finally, it is possible to use the solution of the Sternheimer equation to define the linear-response of the electron localization function (lr-ELF) – a quantity that can be used to help understanding electronic excitations in complex systems. All these phenomena are illustrated with benchmark calculations for molecules and clusters.

Time-dependent density-functional theory in the real-time domain: a route to non-linear response properties and ab-initio many-electron Optimal Control theory.

Alberto Castro and E. K. U. Gross

Institut für Theoretische Physik, Freie Universität Berlin

Abstract

We discuss the current state of the art of the explicitly time-dependent formulation of time-dependent density-functional theory (TDDFT). In particular, we present two applications: (i) Non-linear molecular optics, either in the very high-field (non-perturbative) regime, or in the moderate-field regime where TDDFT provides a means to calculate the low-order (magneto)-optical coefficients – i.e. hyper-polarizabilities, second harmonic generation, etc; (ii) Optimal Control Theory (OCT) for many-electrons systems. We present some possible routes, based on real-time TDDFT, to implement the theory of optimal control without making use of simplifying models or having to tackle with the full wave-function. We will show our working computational scheme for OCT – currently utilized for one-electron systems – and work is in the way to extend it to the many electron case.

Structural and optical transitions of the Biliverdin chromophore

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Myrta Grüning^{4,2}, Angel Rubio^{1,2}

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4. *Unité PCPM, Université Catholique de Louvain, Louvain-la-Neuve, Belgium.*

Abstract

Phytochromes constitute a widespread family of photoreceptors found in plants and bacteria, where they act as photomorphogenesis regulators. It is now well-established that they exist in two forms: the P_r , physiologically inactive and absorbing red light, and the P_{fr} , absorbing in the far-red domain. It has also been shown that the P_r - P_{fr} transition mechanism involves an isomerisation process. Yet the actual transition path is still an open question, since it has only been possible to directly observe the P_r form so far, and several models are still being debated.

Biliverdin is the phytochrome found in bacteria, and has been observed as a crystal in its P_r form within the surrounding protein. Its P_r - P_{fr} transition has been studied both experimentally and theoretically. The most involved region of the molecule has been identified, though no definitive answer has been given for the final geometry. The protonation state of the P_{fr} form is not clear either, and the mechanisms of the possible proton transfers occurring are still unknown. Adding to the confusion, recent studies suggest that the transition might involve a rotation around a single bond in addition to isomerisation. Due to steric clashes, this rotation would in turn cause further conformational changes in the protein environment. Until now this process has been eluded because of its complexity.

All these considerations clearly call for a finer-grained theoretical insight, that we aim at providing the experimentalists with. The chromophore itself being composed of a few dozens of atoms, we are able to study it by means of *ab initio* DFT calculations. When adding the protein environment, the number of atoms immediately goes above 1500, requiring a different level of approximation, and we are exploring several available frameworks. In all cases we are evaluating and comparing the possible protonation states, in addition to systematically study the aforementioned single-bond rotation. In order to compare our results with experiments, we calculate the Raman spectra of all the structures we investigate.

Not only will the knowledge of the P_{fr} form give the correct mechanism of the photochemical transition, as it will open the way to the description of the reverse transition (called *dark reversion*), which is orders of magnitude slower and follows obviously a different path. It will then become possible to understand how the metabolic state of the cell, in particular oxygen levels, influence both transitions.

This work is carried out in collaboration with the experimentalists at the Freie Universität Berlin, Pr. R. Bittl, Dr. M. Brecht, and J. Nieder. We gratefully acknowledge support from Nanoquanta, UPV (Arina) and BSC (Mare Nostrum).

First-principles Optical Properties of semiconducting surfaces and nanowires: the role of the excitonic effects

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Abstract

The experimental characterization of nanomaterials and also the ability to invent for them new functionalities, depends heavily on the understanding of their electronic excitations and their dielectric response. Parameter-free calculations of the optical spectra, based on the Density-functional theory (DFT) joined with the many-body perturbation theory (MBPT) have witnessed impressive advances in recent years. Several examples of Bethe-Salpeter calculations in different systems from bulk materials, to surfaces, nanostructures, molecules and liquids, are today present in the literature. In the present speech, after an overview of this theoretical/computational approach, very well known in this community, I aim to concentrate on several applications regarding the surface optical spectra of some semiconducting materials and of Ge and Si nanowires.

Controlling Polarization at Insulating Surfaces: Electron Spectroscopy of Molecules Adsorbed on Thin Epitaxial Films

Christoph Freysoldt, Patrick Rinke, and Matthias Scheffler

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Abstract

The spectroscopic characterization of insulators has long been hampered by the fact that many techniques such as scanning tunneling microscopy or photoelectron spectroscopy require electrically conducting samples. Growing ultrathin films on metals or doped semiconductors apparently offers a simple solution to this problem as electrons can now tunnel to and from the conducting substrate. However, the direct transfer of experimental conclusions from these films to surfaces of macroscopic samples relies on the two critical assumptions that a) the thickness dependence and b) interactions with the substrate are negligible for the adsorption and other surface properties. We have previously shown from a ground state perspective that this is generally not the case [1]. Here we extend the study to include also the spectroscopic perspective for clean and adsorbate-covered insulator films. We present density-functional theory (DFT) and G_0W_0 quasiparticle energy calculations for NaCl/Ge(100) as prototypical insulator/semiconductor system and consider its interaction with CO as model adsorbate.

The NaCl/Ge(100) system has been experimentally studied with a variety of techniques. Using DFT calculations, we have determined its hitherto unknown atomic structure and find good agreement with all experimental observations. For CO adsorbed on NaCl/Ge, we predict by means of G_0W_0 calculations a considerable, substrate-induced reduction of the quasiparticle (HOMO-LUMO) gap by more than 3 eV compared to the gas phase and 1 eV compared to the NaCl surface. As a function of NaCl film thickness the CO gap increases by 0.1-0.2 eV per NaCl layer. The physical origin of this behavior is simple: the charged excitation in the molecule polarizes the underlying NaCl film and the Ge substrate – an effect naturally incorporated in the GW self-energy, but not in standard, local DFT functionals. By varying the thickness of the NaCl film the influence of the substrate polarization on the molecule can be controlled, which would be desirable from a spectroscopic point of view. However, a larger film thickness also comes at the expense of a smaller tunneling current. We expect that the effects reported here are even more pronounced for metal substrates due to their larger polarizability. We also discuss the technical aspects of the G_0W_0 calculations arising from these polarization effects.

[1] C. Freysoldt, P. Rinke, and M. Scheffler, Phys. Rev. Lett., accepted.

Electronic excitations and excited-state forces of the H:Si(001)-(2x1) monohydride surface

M. Rohlfing¹, N.-P. Wang², P. Krueger³, J. Pollmann³

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Abstract

We investigate electronic excitations of the H:Si(001)-(2x1) monohydride surface using first principles approaches. Density-functional theory is used to calculate the ground state geometry of the system. The quasiparticle band structure is calculated within the GW approximation. Taking the electron-hole interaction into account, electron-hole pair states and optical excitations are obtained from the solution of the Bethe-Salpeter equation for the electron-hole two-particle Green function. In this work we focus, in particular, on localized excitations of the silicon-hydrogen bonds at the surface layer. These excitations give rise to an outward-directed force on the hydrogen atoms, which may well explain their optically induced desorption from the surface as observed in recent experiments. The localization of the excitation is described by an additional confinement potential in addition to standard many-body perturbation theory. [1] N.-P. Wang, M. Rohlfing, P. Krueger, and J. Pollmann, Phys. Rev. B 74, 155405 (2006).

Perspectives in RIXS (Resonant Inelastic X-ray Scattering)

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Abstract

RIXS (Resonant Inelastic X-ray Scattering) is receiving increasing attention due to the possibilities offered by the modern x-ray sources allowing high quality measurement. The presentation is divided in two parts. In the first part the basic physics of RIXS is summarized with reference to benchmark cases selected among strongly correlated systems containing 3d-transition elements. Particular attention will be given to L3-edge excitation. The aim of the second part is to stimulate new theoretical work on RIXS since this is highly needed and will have paramount importance. A whole hierarchy of successive approximations in treating RIXS is presented showing that also relatively simple work can be very useful. Moreover the perspectives of more sophisticated work, both experimental and theoretical, are discussed.

BSE and real space multiple scattering approaches to core electron spectroscopy

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Abstract

Due to recent developments in time-dependent density functional theory and many-body perturbation theory, it is now possible to model optical properties of a wide variety of systems quantitatively from first principles. However, similar statements cannot yet be made for core-level spectroscopies. Although in many cases the calculated results are in quantitative agreement with experiment, it is easy to find examples where this is not true.

We discuss here two approaches to core-level spectroscopies. These are the band-structure based Bethe-Salpeter equation (BSE) approach [1], and the real-space multiple scattering approach [2]. At first glance it might appear that these approaches have little in common. However, on closer examination they share many of the same basic ingredients. We briefly review how these approaches account for the dominant many-body effects, e.g. core hole-photoelectron electron interaction and final state quasiparticle corrections. The importance of these effects is clarified with a comparison of the calculated spectrum and non-resonant x-ray Raman scattering (XRS) experiment. In many cases the information available in core-level spectroscopies can be accessed only with the help of first-principles methods. As an example, we discuss recent XRS studies [3] of pure and Al-doped MgB₂. We also mention some recent developments, as well as future challenges in first-principles modeling of core-level spectroscopy.

[1] E.L. Shirley, Phys. Rev. Lett. **80**, 794 (1998); J. A. Soininen and Eric L. Shirley, Phys. Rev. B **64**, 165112 (2001)

[2] A. L. Ankudinov, B. Ravel, J. J. Rehr, and S. D. Conradson, Phys. Rev. B, **58**, 7565, (1998); J. A. Soininen, A. L. Ankudinov, and J. J. Rehr, Phys. Rev. B. **72**, 045136 (2005).

[3] A. Mattila, J. A. Soininen, S. Galambosi, S. Huotari, G. Vankó, N. D. Zhigadlo, J. Karpinski, and K. Hämäläinen, Phys. Rev. Lett. **94**, 247003 (2005); A. Mattila et al., submitted.

CVV Auger spectra by first principles

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Abstract

In core-valence-valence (CVV) Auger decays, a valence electron is emitted from the sample upon filling of an atomic core hole by another valence electron. The resulting spectrum provides information on the environment of the emitting atom and on many-body correlations. For weakly interacting particles, the spectrum is well described by the self-convolution of the single particle density of states. Conversely, Cini and Sawatzky (CS) [1] proposed to compute the density of states of the two interacting holes by a Dyson equation having as kernel the hole-hole interaction, which is commonly taken as a fitting parameter.

We propose a procedure, based on density functional theory (DFT), for the ab initio evaluation of CVV Auger spectra in the framework of the CS model. The single particle density of states is evaluated directly, while other quantities are estimated by evaluating a correction due to environment with respect to a reference atomic calculation. There, the binding energy of the primary electron and the interaction of the two holes are extracted by calculations with constrained occupations. The evaluation of spin orbit contributions, multiplet splitting, and Auger matrix elements, is already well established for the atom. Subsequently, to describe a generic environment, one adds to the energy of screening a correction computed by taking derivatives of the total energy with respect to particle numbers, or equivalently of the DFT eigenvalues.

Results for bulk Zn and Cu will be presented and compared to experiments [2]. The overall agreement is rather good for a parameter free theory, and allows for investigation of environment specific effects.

[1] M. Cini, *Solid State Communications* **24**, 681 (1977); C. A. Sawatzky, *Physical Review Letters* **39**, 504 (1977).

[2] S. P. Kowalczyk, R. A. Pollak, F. R. McFeely, L. Ley, and D. A. Shirley, *Physical Review B* **8**, 2387 (1973).

New advances in time-dependent density functional theory and quantum transport

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Abstract

A new code for fully nonlinear time-dependent density-functional-theory simulations has been written, tested and applied to a variety of phenomena [1]. Excellent and unique results are obtained for a case where photon emission/absorption is negligible: calculations of the "stopping power" of channeled ions in crystals has produced results that resolve long-standing issues and identify the microscopic mechanisms that control the so-called Z1 oscillations. In cases where photon emission/absorption is dominant, the results are mixed and puzzling. A new method has been developed for transport calculations in molecules and nanostructures [2]. The method maps the "open" scattering problem onto a "closed" eigenvalue-like problem. It has been implemented using the newly developed Lagrange function basis sets [3] and converged currents are demonstrated for the first time. Results will be reported for a benzene ring and for carbon-nanotube field-effect transistors.

[1] R. Hatcher, M. Beck, A. Tackett and S. T. Pantelides, submitted for publication

[2] K. Varga and S. T. Pantelides, Phys. Rev. Lett. 98, 076804 (2007).

[3] K. Varga, Z. Zhang, and S. T. Pantelides, Phys. Rev. Lett. 93, 176403 (2004).

Theory of electronic transport in organic crystals

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Abstract

We present a theoretical and numerical description of charge-carrier transport in organic molecular crystals. Our approach is based upon a rigorous evaluation of the Kubo formula for electrical conductivity within a mixed Holstein-Peierls model, i.e. including local and nonlocal electron-phonon interaction. Explicit formulas for the polaron bandwidths and mobilities as a function of temperature are derived. The theory is supplemented by ab initio calculations of the relevant material parameters (transfer integrals, electron-phonon coupling, phonons) for various materials (oligo acenes, durene, guanine). The resulting predictions for the electron and hole mobilities show a remarkably good agreement with experiments and provide new insight into several hitherto poorly understood transport phenomena such as the differences between electrons and holes, the peculiar algebraic temperature dependences, and anisotropy effects.

Maximally-Localised Wannier Functions as Building Blocks of Electronic Structure

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Abstract

We combine large-scale, ab initio electronic structure calculations and the maximally-localised Wannier function (MLWF) approach in order to study the electronic properties of complex nanostructures. MLWFs provide an accurate, localised, minimal basis set in which to diagonalise the Hamiltonian. In the MLWF basis, Hamiltonians for large, complex systems can be constructed directly from the short-ranged Hamiltonians of smaller constituent units by performing full first-principles calculations on either periodically-repeated or isolated fragments. We apply our approach to the case of DNA helices. The effects of sequence, twist-angle, and solvation environment on the electronic structure are investigated. This work opens the way to obtaining a more detailed understanding of charge transport and conductance in DNA, bringing closer the prospect of engineering its electronic structure for use in nano-electronic circuits and biotechnology applications.

Many-body effects and inelastic electronic transport through nanoscale devices

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¹ *Department of Physics, University of York, York YO10 5DD, UK;* ² *CEA-Saclay, DSM/DRECAM/SPCSI, B.462, F-91191 Gif-sur-Yvette, France.*

Abstract

We consider the problem of interaction between particles (electrons e and phonons ph) in the context of electronic transport in nanoscale devices. We present a technique based on non-equilibrium Green's functions and include the many-body effects under the form of self-energies. Different levels of approximation are used to determine the corresponding e - e and e - ph self-energies.

We apply this technique to model systems describing a lead-molecule-lead heterojunction and calculate both the current and current-current correlation functions.

We show that, for the e - ph interaction, it is necessary to go beyond the commonly-used self-consistent Born approximation (SCBA) to obtain correct results for a wide range of parameters. We also discuss the fluctuation-dissipation theorem in the context of non-equilibrium transport. Finally, we briefly consider the calculation of different self-energies for the e - e interaction (HF,GW, etc.) and their extension to the non-equilibrium case.

The conductance and polarizability of nanostructures

Matthieu Verstraete, Peter Bokes, and Rex Godby

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Abstract

We present ab-initio and tight binding results for the conductance of nanowires. Our formalism extracts the transport properties directly from the non-local polarizability, giving an intrinsic characterization of the device, without leads. The system-size and temperature dependencies are examined and show non-trivial behavior, in particular in a periodic supercell setup. This method is ideally suited to incorporation in standard ground- and excited-state electronic structure methods, irrespective of basis set and implementation details.

TDDFT in Molecules and Polymers for photovoltaic applications

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Abstract

The search of new types of polymers with specific physical properties such as the optical gap is of great interest to better address applications like photovoltaic devices. Electronic structure calculations can help in the design of new polymers by identifying the most promising candidates, and in this respect, being able to accurately compute optical gaps is crucial. One particular class of polymers of interest is the ladder-type polymers. These have more than one bond linking the neighboring monomers together, eliminating the possible dihedral degree of freedom. These polymers are known generally to exhibit small band gaps, due partly to their planar configurations which maximize the alignment of the π orbitals. Moreover, these ladder-type polymers have the potential to exhibit very high intrachain mobility. In this presentation, we will report the results of time-dependant density-functional theory (TDDFT) calculations with both the PBE and B3LYP functionals on ladder-type polymers which include hetero-atoms like B, C, N, Si, P, S, Ga, Ge, In, Sn and Hg. The oscillator strength of these different polymers will also be address.

Long-range and Long-Chain Molecules in TDDFT: Modelling the exact kernel

Neepta T. Maitra

Hunter College of the City University of New York

Abstract

Recent years have witnessed increasingly wide and varied applications of TDDFT for excitations and response. We discuss why the usual approximations fail in certain cases involving double excitations, long-range charge transfer excitations, and polarizabilities and dissociation of long-range molecules, and derive model kernels to try to fix these problems.

Temperature effects in the optical response of clusters using time dependent density functional theory

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Abstract

Many properties of atomic clusters are known to be size-dependent, *e.g.*, the structural and optical properties. There are, however, factors other than size that can play an important role in determining the properties of nano-scale systems. Temperature, in particular, has been shown to have a strong effect on the optical response of open-shell sodium clusters. I will illustrate an approach to incorporate the role of temperature in the optical absorption spectra of sodium clusters by combining pseudopotentials, Langevin molecular dynamics and time-dependent density functional theory. I will also present a new computational procedure to address the electronic structure of large systems based on a real space implementation of pseudopotentials.

- [1] I. Vasiliev, S. Ögüt, and J.R. Chelikowsky: “*Ab Initio* Excitation Spectra and Collective Electronic Response in Atoms and Clusters,” *Phys. Rev. Lett.* **82**, 1919 (1999).
- [2] L. Kronik, I. Vasiliev and J.R. Chelikowsky: “*Ab initio* Calculations for Structure and Temperature Effects on the Polarizabilities of Na_n ($n \leq 20$) Clusters,” *Phys. Rev. B* **62**, 9992 (2000).
- [3] J.R. Chelikowsky, L. Kronik and I. Vasiliev: “Time dependent density functional calculations for the optical spectra of molecules, clusters and nanocrystals,” *J. Phys. Cond. Matt.* **15**, R1517 (2003).
- [4] I. Vasiliev, S. Ögüt, and J. R. Chelikowsky: “First Principles Density Functional Calculations for Optical Spectra of Clusters and Nanocrystals,” *Phys. Rev. B* **65**, 115416 (2002).
- [5] M. Lopez del Puerto, M.L. Tiago, and J.R. Chelikowsky, “*Ab initio* calculation of temperature effects in the optical response of open-shell sodium clusters,” *J. Chem. Phys.* (2007), in press.

Macroscopic limit of time-dependent density-functional theory for adiabatic local approximations of the exchange-correlation kernel

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Abstract

Time-dependent density-functional theory (TDDFT) is a rather accurate and efficient way to compute electronic excitations for finite systems. However, in the macroscopic limit (systems of increasing size), for the usual adiabatic random-phase, local-density, or generalized-gradient approximations, one recovers the Kohn-Sham independent-particle picture, and thus the incorrect band gap. To clarify this trend, we investigate the macroscopic limit of the exchange-correlation kernel in such approximations by means of an algebraical analysis complemented with numerical studies of a one-dimensional tight-binding model. We link the failure to shift the Kohn-Sham spectrum of these approximate kernels to the fact that the corresponding operators in the transition space act only on a finite subspace [1]. Finally we discuss how an analysis similar to the one in this work can be applied to more sophisticated approximations for the kernel like the expressions derived from many-body perturbation theory.

[1] M. Grüning and X. Gonze PRB 76 (scheduled issue 7, 15 august)

Towards an Exact Treatment of Exchange and Correlation in Materials

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Abstract

Recent studies have shown that the errors of present-day exchange-correlation functionals, for example LDA and GGA, are rather short ranged.[1-3] For extended systems, *the correction* to LDA can therefore be evaluated by properly chosen clusters and employing highest-quality quantum chemistry or quantum Monte Carlo methods. This approach is applicable to bulk systems as well as to defects in the bulk and at surfaces.

In particular we address in this talk LDA and GGA errors due to self-interaction and due to the lack of van der Waals interactions. Furthermore, for the description of metallic bulk systems our study reveals the problematic performance of Hartree-Fock, MÅller-Plesset perturbation theory, and of the popular B3LYP functional.

[1] Q.-M. Hu, K. Reuter and M. Scheffler, Phys. Rev. Lett. 98, 176103 (2007).

[2] C. Filippi, S.B. Healy, P. Kratzer, E. Pehlke, and M. Scheffler, Phys. Rev. Lett. 89, 166102 (2002)]

[3] C. Tuma and J. Sauer, Chem. Phys. Lett. 387, 388 (2004); Phys. Chem. Chem. Phys. 8, 3955 (2006).

The bandgap within reduced density matrix functional theory

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Abstract

Reduced-density-matrix-functional theory (RDMFT) uses the one-body density matrix as basic variable instead of the density which is used in DFT. The eigenvalues of the one-body density matrix are known as occupation numbers while its eigenfunctions are called natural orbitals. In practical calculations, the variation of the total energy with respect to the one-body density matrix is replaced by a variation with respect to the occupation numbers and the natural orbitals.

Within RDMFT it is possible to calculate the fundamental gap (i.e. the band gap in case of periodic systems) as the discontinuity of the chemical potential as a function of the particle number. Using this method for finite systems yields results which are in very good agreement with CI calculations and experimental data. For the application of RDMFT to periodic systems one has the choice of describing the natural orbitals either as Wannier- or as Bloch states. We discuss the consequences of both choices and present numerical results for one- and three-dimensional systems.

Edge-induced spin Hall effect in a clean 2D homogeneous electron gas

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Abstract

We analyze the importance of the confining potential close to the edge of the electronic system on the spin Hall effect in a 2D homogeneous electronic gas. We show that in similarity with the extrinsic spin Hall effect, the spin-orbit interaction and the current flow induce accumulation of the out of plane up and down spin density on the right and left edge of the system respectively. We quantify the amplitude and spatial extent of the uncompensated spin density for a system exhibiting the conventional spin Hall effect. While the amplitude of the spin accumulation is comparable to the experimental values, the spatial extent of the spin accumulation due to the edge is restricted to the distances of the order of Fermi wavelength (cca 10nm). Simplicity of the system allows for a full non-perturbative treatment within the Green's function formalism for variable temperature, current density, and the amplitude of the confining potential.

Breakdown of the adiabatic approximation in a doped graphene monolayer and in metallic carbon nanotubes

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Abstract

We compute, from first-principles, the frequency of the phonons associated to the Raman G bands in a graphene monolayer [1] and in metallic nanotubes [2] as a function of the charge doping. In both cases, the frequency displays an important measurable shift in the range of doping reached experimentally. As a consequence, Raman spectroscopy can be used as a direct probe of the doping of these systems [3]. Calculations are done using i) the adiabatic Born-Oppenheimer approximation and ii) time-dependent perturbation theory to explore dynamic effects beyond this approximation. The two approaches provide very different results. The frequency shift of the G band in graphene and of the G- in metallic tubes represent remarkable failures of the adiabatic Born-Oppenheimer approximation.

[1] M.Lazzeri, F.Mauri, Phys. Rev. Lett. 97, 266407 (2006)

[2] N. Caudal, et al. Phys. Rev. B 75, 115423 (2007).

[3] S.Pisana et al. Nature Materials 6, 198 (2007).

Quantum transport in “real” carbon nanotubes

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Abstract

Carbon Nanotubes (CNTs) are constantly attracting the interest of researchers because they offer the opportunity of investigating fundamental physical properties at the nanoscale and being exploited as building blocks for nanoelectronic devices. Among the different possible applications of CNTs, the present work focuses on their use as nanosensors for gas detection thanks to the change in conductance of the nanodevice in presence of the gas to be detected. To reach this goal, the structural, electronic and transport properties of CNTs have been investigated for perfect tubes, tubes containing defects such as vacancy, di-vacancy, oxygenated vacancy, and tubes decorated with metal clusters.

Due to the “nano” size of the systems under investigation, atomistic simulations become necessary for an accurate modelling of their structural, electronic, and transport properties. Indeed, effective bulk parameters cannot be used for the description of the electronic states since interfacial properties play a crucial role and semiclassical methods for transport calculations are not suitable at the typical scales where the device behavior is characterized by coherent tunnelling. Consequently, quantum-mechanical computations with atomic resolution can be achieved using localized basis sets for the description of the system Hamiltonian and can predict electronic and transport properties of nanostructures.

In the present work, the structural and electronic properties of CNTs are obtained via the *ab initio* method as implemented in the SIESTA code, *i.e.* the calculations are based on density functional theory (DFT), using norm-conserving pseudopotentials (Troullier-Martin) and atomic orbitals basis set. The quantum conductance of the system is achieved from electronic transport calculations performed with the SMEAGOL code. The latter is based on the non-equilibrium Green’s function (NEGF) formalism and uses the one-particle Hamiltonian obtained from the DFT calculations. Such approach, which combines NEGF and DFT, allows us to model real systems constituted by hundreds of atoms to a high degree of accuracy.

Many-body corrections and optical properties of graphene nanoribbons

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Abstract

Recent advances in the synthesis of single layered graphite [1-3] have focused the attention on novel quasi-one-dimensional carbon-based systems, i.e. graphene nanoribbons (GNRs) [4,5]. In particular, the possibility of patterning graphene sheets in a controllable manner opens exciting opportunities for future nanoscale optoelectronics applications. One of the most interesting features of these systems is the sensitivity of their properties to the ribbon-edge shape [6,7], which dictates the classification of GNR in armchair (A), zigzag (Z) or chiral (C) ones. Here we focus our attention on A-GNRs, which can be further classified in three distinct families: $N=3p+1$, $N=3p$, $N=3p+1$, where N indicates the number of dimer lines across the ribbon width. In particular, we calculate the optical spectra of nanometer-sized A-GNRs belonging to different families and with different edge terminations, namely hydrogen-passivated and clean-edge ribbons. As in the case of other one-dimensional systems, the spatial confinement is expected to induce a strong enhancement of Coulomb interactions. The resulting many-body effects are fully accounted within the GW-BSE scheme [8]. Indeed, in all the studied cases, the inclusion of many-body corrections is shown to be crucial in determining both the peak position and its lineshape, and the optical spectra are always dominated by strongly bound excitons. Besides, we find a significant dependence of both the energy gap and binding energy on the ribbon family. This, together with the edge termination, also determine the presence of optically inactive excitonic states, thus affecting the luminescence efficiency.

- [1] K. S. Novoselov et al., Nature 438, 197 (2005).
- [2] Y. Zhang et al., Nature 438, 201 (2005).
- [3] C. Berger et al., Science 312, 1191 (2006).
- [4] Z. Chen et al., condmat/0701599 (2007).
- [5] M. Y. Han et al., Phys. Rev. Lett., 98, 296805(2007).
- [6] Y. Son et al., PRL 97, 216803 (2006).
- [7] V. Barone et al., Nano Lett. 6, 2748 (2006).
- [8] G. Onida et al., Rev. Mod. Phys. 74, 601 (2002).

A First-Principles Approach to Designing Materials

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Abstract

The role of basic energetic and thermodynamic data in designing new materials is crucial towards their application. Fundamental knowledge of the microscopic factors governing alloy phase stability has increased greatly due to the development of highly accurate state-of-the-art first principles computational approaches and recent works have demonstrated substantial quantitative improvements in the accuracy of alloy phase diagrams calculated by these techniques. Our presentation will be illustrated by applications to the modelling of phase diagrams in Pu- based alloys and the structural stability of UO₂ under irradiation.

Superconducting transition in doped diamond and silicon

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Abstract

After introducing the field by presenting the case of the doped silicon clathrates [1], we study the superconducting transition in highly-doped diamond [2] and silicon [3]. Both experimental and theoretical aspects will be overviewed. At large boron doping, that is beyond the Mott metal-insulator transition, diamond and silicon have been shown to become superconducting with a T_C up to 10 K in the diamond case. The study of the electronic properties and electron-phonon coupling strength λ allows to identify the modes responsible for the superconducting transition and provides support to a standard BCS mechanism, even though some questions remain opened concerning the value of the Coulomb repulsion parameter μ^* and the relation between the doping rate and T_C . Strategies to increase T_C are discussed. Increasing the boron content in diamond may not be so efficient as boron tend to cluster in electronically inactive dimers [4]. In the case of silicon, changing boron by aluminum is shown to enhance T_C by one order of magnitude, an effect due to a negative pressure effect [5].

[1] "Superconductivity in doped sp³ semiconductors: the case of the clathrates", D. Connetable et al., Phys. Rev. Lett. 91, 247001 (2003).

[2] "Role of the Dopant in the Superconductivity of Diamond", X. Blase, Ch. Adessi, D. Connetable, Phys. Rev. Lett. 93, 237004 (2004).

[3] "Superconductivity in doped cubic silicon", E. Bustarret, C. Marcenat, P. Achatz, J. Kacmarcik, F. Levy, A. Huxley, L. Ortega, E. Bourgeois, X. Blase, D. Debarre, J. Boulmer, Nature (London) 444, 465-468 (2006).

[4] "Impurity dimers in superconducting B-doped diamond: Experiment and first-principles calculations", E. Bourgeois, E. Bustarret, P. Achatz, F. Omnes, X. Blase, Phys. Rev. B 74, 094509 (2006).

[5] "Superconductivity in doped cubic silicon: an ab initio study", E. Bourgeois and X. Blase, Appl. Phys. Lett. 90, 142511 (2007).

Analysis of the Difference between All-Electron and Pseudopotential Based G_0W_0 Calculations

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Abstract

In recent years, the GW approach, typically applied as a first order correction to the Kohn-Sham (KS) eigenvalues (G_0W_0 approximation), has achieved great success in describing single-particle excitations in weakly correlated semiconductors and insulators [1]. For implementation simplicity and computational efficiency, most of the existing codes are based on the pseudopotential (PP) method, in which the self-energy is calculated only from the pseudo-valence states. It is well-known in DFT that such a linear treatment of the core-valence exchange-correlation interaction is not always valid. Although within PP- G_0W_0 the core-valence interaction can only be included at the KS level, its reported results usually show a better agreement with experiment than the all-electron calculations available so far [2-4].

The reasons for this disturbing discrepancy can be traced back to two approximations underlying the PP- G_0W_0 , namely, the exclusion of the core electrons in the calculation of the self-energy (core-valence linearization) and the use of pseudo-valence wave functions (pseudoization). We calculated the G_0W_0 corrections to the band gaps for a set of materials (e.g. Si, GaAs, NaCl, AlP, ...) using both all-electron- and PP- G_0W_0 . The all-electron calculations are performed using our recently developed G_0W_0 code based on the Wien2k implementation of the FP-(L)APW+lo method. By removing the core states in the all-electron G_0W_0 calculation, we can analyze separately the effects of core-valence linearization and pseudoization. Our results show that the effect of core-valence linearization alone does not explain the difference between all-electron- and PP- G_0W_0 calculations. The effect of pseudoization turns out to be important as well. For materials composed by elements in the second and third rows of the periodic table, like Si and AlP, it even is the dominant reason for the better agreement between PP- G_0W_0 calculations and experiments. For material including very shallow d states, like GaAs, the core-valence linearization is dominant. To avoid these errors, all-electron results have to be taken as benchmark in G_0W_0 calculations.

Electronic correlation in 3d transition metals beyond *GW*: The FLEX method

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Abstract

The *GW* approximation (GWA) has evolved as the state of the art for ab initio calculations of electronic excitations and spectroscopies. For large classes of materials, especially semiconductors and simple metals, quasiparticle spectra calculated within the GWA are in very good agreement with experiments. However, it ignores spectral features resulting from higher-order correlation effects in the localized 3d orbitals of transition metals, such as the famous 6 eV satellite in the photo emission spectrum of nickel. Furthermore, exchange splittings and 3d valence band widths often deviate from experimental measurements. The FLEX (fluctuation exchange) method is a diagrammatic technique describing additional two-particle scattering processes in materials with intermediate correlation strength. By explicitly including multiple scattering in the electron-electron and electron-hole channels, the FLEX method captures correlation effects beyond those contained in the GWA. We have developed a simplified FLEX implementation designed to describe electronic correlation in 3d transition metals. First, density-functional calculations are performed using the full-potential linearized augmented plane-wave scheme. The FLEX method is then applied as a perturbative correction to include two-particle correlation effects in the self-energy of the 3d electrons. The resulting equations are solved self-consistently within the framework of dynamical mean-field theory. We have applied this scheme to selected non-magnetic and ferromagnetic transition metals and present illustrative results.

Including Spin in the Bethe-Salpeter Equation: Excitonic Effects in the Antiferromagnet MnO

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Abstract

Over the past years there was impressive progress in calculating optical spectra of semiconductors beyond the random-phase approximation. The Bethe-Salpeter equation (BSE) was solved to take into account two-particle interactions, especially excitonic and local-field effects. We focus on the problem of calculating optical spectra for systems where spin plays an important role. Therefore, we generalize the BSE with respect to the spin degree of freedom in order to deal with magnetic systems. Prominent examples for spin-polarized materials are antiferromagnets, e.g. transition metal monoxides. Although transition metal oxides are usually considered as the standard test systems for magnetic solids, they are hard to treat numerically. We present explicit results for MnO as the best natured example.

The main difficulty arises from the circumstance that in spin-polarized systems the separation between triplet and singlet excitons no longer holds. Both submatrices of the two-particle Hamiltonian are coupled by the matrix elements of the bare Coulomb potential which account for local-field effects. The numerical cost for the calculation of optical spectra increases due to doubling of the rank of the corresponding eigenvalue problem.

The ground state calculations are performed with a density-functional plane-wave code using the projector-augmented wave (PAW) method for the description of wave functions. Quasiparticle shifts are added to obtain correct gap values. The BSE is solved applying both, direct diagonalization and a time-development scheme.

The electron spin degree of freedom in the calculation of excited-state properties.

F. De Fausti, A. Marini, M. Palummo, C. Hogan, R. Del Sole.

Department of Physics of the University of Rome 'Tor Vergata'

Abstract

The inclusion and proper description of the electron spin is central to the physics of all magnetic materials, ranging from paramagnetic atoms and molecules, to collinear systems such as ferromagnet and non-collinear systems. To study physical phenomena involving excited states, it is often necessary to include many-body effects through Green's function theory or time dependent DFT, although state-of-the-art approaches are still based on DFT calculations as a first approximation. In this presentation, I will show how we have implemented the spin degree of freedom in Many Body Perturbation Theory. First applications are focused on bulk GaSb, which has a large spin-orbit splitting (0.8 eV) and therefore should be treated in a non-collinear framework. We have calculated the self-energy corrections to the spin-orbit electronic band structure within the GW approach and carried out the solution of the Bethe-Salpeter equation, as required for an appropriate description of the electron-hole interaction.

Optical properties of ZnO – the influence of strain and spin-orbit coupling

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Abstract

Zinc oxide is a material of scientific interest since many decades with a wide range of applications. As an environmentally friendly material with interesting optical properties it is a possible candidate for substituting GaN in optoelectronic applications in the blue/ultraviolet region. It can be grown as high-quality single-crystals. [1] Also for ab-initio calculations ZnO is an interesting material – mainly due to difficulties in the description of the shallow semicore d-electrons. The band-ordering at the valence band maximum is subject to discussions in the literature. We study excitonic effects in the optical spectra and especially bound excitons at the absorption edge by solving the Bethe-Salpeter equation together with a perturbative treatment of spin-orbit coupling. To reduce the size of the emerging huge excitonic Hamiltonian matrices we use hybrid k-point-meshes which allows us to compute converged and highly accurate results in the range of meV. Biaxial strain is considered as a possible reason for contradicting experimental results for the valence band ordering. We also compute the dielectric function up to 23 eV and compare with experimental results. The influence of QP energies on the spectrum is discussed.

[1] C. Klingshirn, ChemPhysChem 8, 782 (2007)

Conserving exchange-correlation potentials and response kernels in spherical atoms

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Abstract

In this work we have studied a few different, so called, Φ -derivable or conserving approximations for the electron-electron interaction in the framework of time-dependent density functional theory (TDDFT). For some spherical atoms the exchange-correlation (XC) potential v_{xc} , corresponding to the GW approximation to the total energy is presented and compared to that of the exact exchange approximation and the second order or MP2 approximation. In addition, the XC kernel in exact exchange has been calculated, including the full frequency dependence. This kernel has then been used to calculate a number of physical properties like, *e.g.*, total energies and polarizabilities. Some attention is given to our use of cubic splines as radial basis functions, which have shown to be numerically stable and very accurate.

Time-dependent density-functionals from non-equilibrium Green function theory

Robert van Leeuwen, Nils Erik Dahlen, Adrian Stan

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Abstract

In this presentation we will present a general method to construct time-dependent density functionals from many-body perturbation theory. These functionals can be constructed in such a way that they display a number of physically desirable features such as the satisfaction of macroscopic conservation laws and the inclusion of memory effects. These features are essential for a good performance of density functionals for quantum transport phenomena which involve strong fields and dissipation. The tools to construct these functionals are based on the elegant techniques of nonequilibrium Green function theory. We also solved the Kadanoff-Baym equations for the nonequilibrium Green function which can serve as an important benchmark for new approximate density functionals and will also give valuable insight into the importance of electronic correlations in the transport problem.

The GW and the Time Dependent GW Approximations for Nonequilibrium Systems

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Abstract

The formalism of Nonequilibrium Green Functions Theory is used to investigate the role of electron correlation in several types of systems. Various "GW-like" approximations are studied in detail for inhomogeneous nonequilibrium systems. The importance of the using both full self-consistency and conserving approximations, is underlined. We also apply the Kadanoff-Baym equations to nonequilibrium inhomogeneous systems within time dependent GW and we discuss the equivalence of this approach to the solving of the Bethe-Salpeter equation with highly advanced kernels.

Defects in semiconductors and their optical spectra

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Abstract

Point defects in semiconductors, like dopant impurities, lattice vacancies or interstitials, represent the smallest conceivable nanoscale perturbations of an otherwise ideal three dimensional lattice. Their localized electronic states within the fundamental band gap enabled the design of electronic devices without which our daily life would have been drastically different. Naturally much effort has been dedicated to the investigation of the nature of the point defects and their kinetics. The position of the defect levels within the band gap and optical excitations of the defect electrons are defect fingerprints typically used for the defect characterization. Other important fingerprints characterized in experiments are localized vibrational modes and the hyperfine tensors that describe the interaction of the spin of a localized defect electron with the nuclear spin of the surrounding atoms. The quantitative prediction of the latter fingerprints by density functional theory (DFT) in conjunction with the local density approximation (LSDA) enabled recently the identification of fundamental defect centers and defect complexes in Silicon Carbide. On the other hand, the evaluation of defect levels is affected by the well known DFT band gap error and finger prints of the excited state cannot be assessed on rigorous grounds in a ground state theory. On the basis of many body theory we address these defect fingerprints making use of the GW approximation and including excitonic effects by solving the Bethe-Salpeter equation. We apply this approach to the carbon vacancy in SiC. The current interpretation of optical experiments on this center indicates in contrast to general expectation and the results of DFT-LDA theory that Frank-Condon shifts should be negligible. Inclusion of quasiparticle and excitonic effects beyond the DFT-LSDA picture does not resolve the discrepancies, but rather suggest a different interpretation. The presentation briefly reviews the major achievements in the identification of point defects and their clusters in SiC and exemplarily addresses the optical excitation of the carbon vacancy.

Exciton-Phonon coupling in the finite temperature optical absorption of semiconductors

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Abstract

The description of excitonic states based on the Ab-Initio Bethe-Salpeter equation (BSE) constitutes an efficient and successful tool to calculate the optical properties of a wide range of electronic systems[1]. Nevertheless the state-of-the art implementation of the BSE neglects the contribution of the nuclear motion that is crucial to explain the temperature dependence of the optical absorption[2] and to correctly account for the zero point motion effect in the zero temperature limit[3]. Moreover, the observation of phonon sidebands in the photoluminescence (PL) spectra[4], or the time-decay of excitons in time-resolved PL[5] suggest a new, dynamical picture of the excitonic states induced by the exciton-phonon scatterings. This is the goal of the present work: to derive an extension of the (dynamical[6]) BSE the include exciton-phonon coupling, either indirect (quasiparticle mediated) or direct, corresponding to an additional four point phononic kernel. The exciton-phonon BSE will then be applied to the finite temperature spectra of semiconductors with resonant and bound excitons. I will discuss how the exciton-phonon coupling correctly describes the zero-point motion effect, the excitonic damping, the finite temperature effects and the phononic sidebands.

[1] G.Onida, L.Reining and A.Rubio, *Rev. Mod. Phys.* **74**, 601 (2002).

[2] P. B. Allen and M. Cardona, *Phys. Rev. B* **27**, 4760 (1983), and references therein.

[3] P. Lautenschlager, M. Garriga, L. Vina, and M. Cardona, *Phys. Rev. B* **36**, 4821 (1987).

[4] V. Perebeinos, J. Tersoff, and P. Avouris, *Phys. Rev. Lett.* **94**, 027402 (2005).

[5] A. Hagen, et. al., *Phys. Rev. Lett.* **95**, 197401 (2005).

[6] A. Marini, R. Del Sole, *Phys. Rev. Lett.*, **91**, 176402 (2003).

Efficient Calculations of Electronic Excitations with a Localized GW Formalism

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Abstract

First principles predictions of the electronic excitations of molecules, clusters, and/or molecules adsorbed on surfaces are very important from both a theoretical and a technological point of view. Many-body perturbation theory within Hedin's GW approach is a successful framework for this task, and is frequently applied to study periodic systems. However, GW studies of finite systems are still the exception. This is due to the fact that most GW implementations utilize plane-wave basis sets. The periodic boundary conditions impose a supercell geometry whose required size typically renders the computational cost prohibitively expensive for finite systems. It is the goal of the present work to develop a GW formalism using a localized basis set, which by construction promises to give an efficient, all-electron description of the excitations of both confined and extended systems on equal footing.

Our GW formulation is based on a new efficient DFT code FHI-aims [1], in which numeric atom-centered orbitals are employed as basis functions. As a first application, we have studied a set of finite systems spanning individual atoms, small molecules (methane, silane, benzene), small clusters (Na_n), and biomolecules (alanine). In all cases, we performed G_0W_0 calculations, in which GW is applied as a perturbation to an underlying ground-state calculation. Our approach requires only a moderate amount of basis functions, which considerably increases the efficiency compared to plane-wave based approaches. A key feature of our GW formalism is that intermediate quantities like the polarizability and the screened Coulomb potential are represented by a second, auxiliary set of atom-centered basis functions. Thanks to the resolution of identity technique, the same auxiliary basis functions enable us to do Hartree-Fock (HF), and hence hybrid functional calculations on the same platform. For all our test cases G_0W_0 produces ionisation potentials in much better agreement with experiment compared to LDA, HF or hybrid functionals. By applying G_0W_0 separately as perturbation to LDA (strong self-interaction) and HF (self-interaction free, but no correlation) we can systematically investigate the mechanism behind this improvement. As implied by its construction, G_0W_0 reliably removes the self-interaction present in the ground state and adds correlation resulting from the electronic screening. It thus significantly reduces the spread in the single particle levels of the ground state calculation [severe under (over)estimation in LDA (HF)] with only a small residual starting point dependence remaining.

[1] V. Blum *et al.*, *The FHI Ab Initio Molecular Simulations (aims) project*, Fritz-Haber-Institut, Berlin (2007).

GW band-structure and self-energy real-space decay by means of maximally-localized Wannier functions.

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Abstract

The use of maximally localized Wannier functions (MLWFs) [1] recently became very popular in the electronic structure community, as a supplementary analysis tool. On one hand, MLWFs are attractive because they constitute a localized basis set which is complete and orthonormal, while on the other hand, they also carry physical information. Among the many properties of WFs once they are adopted as a basis, it is possible to exploit the real-space decay of the periodic Hamiltonian operator to refine its spectrum in terms of a better sampling of the Brillouin zone (BZ). This feature is particularly appealing in those cases where dealing with a large number of \mathbf{k} -points is expensive, like *e.g.* the GW method.

In this work we show that BZ interpolation using MLWFs is feasible also in the case of the quasi-particle (QP) calculation within the GW approximation. We apply the method to silicon bulk as a test case, as well as to realistic systems like polymer crystals and quartz. The computed QP-band structures are in good agreement with reference data, where available. We also discuss and compare the real-space decay of the GW self-energy in the analyzed cases.

All the calculations have been performed using the WANT package [2] to compute MLWFs and the SAX code [3] for the GW corrections.

[1] N. Marzari, and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997).

[2] WANT project, <http://www.wannier-transport.org>.

[3] SAX project, <http://www.sax-project.org>.

Wannier function approach to electron correlation in transition metals

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Abstract

First-principles calculations of quasiparticle energies in real materials are typically based on the *GW* approximation (GWA), which is known to produce good results for systems with weak or intermediate correlation strength. However, it fails to describe short-range interactions in more strongly correlated systems and does not contain spin fluctuations that play an important role in the transport and thermodynamic properties of magnetic materials. In order to treat such local correlations in transition metals and rare earths we develop a computational method that goes beyond the GWA by including appropriate vertex corrections in the form of a multiple-scattering T-matrix, which describes the coupling of electrons and holes with different spins. To reduce the numerical cost for the calculation of the four-point T-matrix we exploit a transformation to maximally localized Wannier functions that takes advantage of the short spatial range of the electronic correlation in the partially filled *d* or *f* orbitals of magnetic materials. Our implementation is based on the all-electron full-potential linearized augmented plane-wave (FLAPW) method. As a first step, we calculate the dynamical spin susceptibility of the non-interacting Kohn-Sham electrons and the matrix elements of the Coulomb potential in the Wannier basis. The obtained values for the latter agree with previous calculations.

Understanding correlations in VO₂: self-consistent quasiparticle calculations and alternatives

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Abstract

Vanadium dioxide (VO₂) is a prototype material for the discussion of correlation effects in solids. Here we present a parameter-free GW calculation of VO₂ and show that correlation effects in the photoemission spectra of both the metallic and the insulating phases of VO₂ are correctly reproduced, provided that quasiparticle energies and wavefunctions are calculated self-consistently [1]. These calculations are computationally demanding and one is naturally lead to look for possible alternatives. In fact, spectra are derived from contractions of many-body Green's functions. So one calculates more information than needed. We hence illustrate an in principle exact alternative approach to construct effective potentials and kernels for the direct calculation of electronic spectra [2]. In particular, a dynamical but local and real potential yields the spectral function needed to describe photoemission. We discuss for model solids the frequency dependence of this "photoemission potential" stemming from the nonlocality of the corresponding self-energy.

[1] M. Gatti, F. Bruneval, V. Olevano, and L. Reining, submitted to Phys. Rev. Lett. (2007).

[2] M. Gatti, V. Olevano, L. Reining, and I.V. Tokatly, Phys. Rev. Lett. **99**, 057401 (2007).

Mobility gap of silica: many-body contribution

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Abstract

Silica is one of the central material in a wide range of technological applications, for instance, in the MOS governing modern electronic devices. In the recent past, with the advent of nanodevices, the reduced dimensions of the oxide layers and the required abruptness of the interface demands for an atomic-scale understanding of the microscopic processes governing electronic performances, such as the carrier mobility and energy levels. In amorphous semiconductors and insulators the free-carrier transport is directly related to the so-called mobility gap, that is defined as the energy difference between mobility edges, separating localized states tails from extended band states, and plays the same role of the electrical energy gap in crystalline systems. Although extensive studies have been carried out for silica, the experimental values reported in the literature for the measured mobility gap range from 8.8 to 11.5 eV. Under the theoretical point of view, numerical studies have been performed on particular silica polytypes using mainly mean-field approaches or model Hamiltonian. and only very recently a first-principles method based on many-body perturbation theory has been applied to study the optoelectronic of quartz[1] and cristobalite[2]. In any case, no unified physical picture linking density, mobility gaps and disorder has emerged. In the present work, we go beyond the previous studies by using a multi-scale methodology, which comprises generation of reasonably large silica models and calculation of quasi-particle electronic structure by means of the GW approach, through a state-of-the-art first-principles technique within many-body perturbation theory. We performed such calculations for quartz, cristobalite and different glass configurations with different amount of disorder. We find that as expected, disorder introduces localized states in the gap of silica, however the mobility gap is only very weakly influenced by such defects. We also find that, the local fluctuations of the density is responsible for the unexpected high many-body correction in amorphous silica.

[1] E. K. Chang and M. Rohlfing and S. G. Louie, Phys. Rev. Lett. 85, 2613 (2000)

[2] L. E. Ramos and J. Furthmuller and F. Bechstedt, Phys. Rev. B 69, 85102 (2004)

Second order harmonic generation in crystalline semiconductors

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Abstract

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 within the Time Dependent Functional Theory (TDDFT). For cubic symmetries, we show how this approach can be simplified and expressed in terms of the second order response function and of the dielectric function. Numerical results will be presented for SiC and GaAs.

Approaching ground state Born-Oppenheimer molecular dynamics in a modified time-dependent density functional theory approach

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Abstract

To mimic ground state Born-Oppenheimer molecular dynamics (gsBOMD), we propose a Lagrangian inspired by Ehrenfest dynamics in time-dependent density functional theory (TDDFT). The electronic orbitals are evolved by a time-dependent Schrödinger-like equation, where the time derivative of the orbitals is multiplied by a parameter μ , which controls, similarly to Car-Parrinello (CP) dynamics, the time scale of the fictitious electronic motion. The approach presented here automatically preserves the orthonormality of the orbitals and conserves the total physical energy for all values of μ . We show that the new dynamics smoothly approaches gsBOMD in the $\mu \rightarrow 0$ limit as expected, and that it remains close to it along a wide range of values of $\mu > 1$. As in CP, there is a compromise between the time-step (TS) and the closeness to gsBOMD given by the value of μ . These properties are illustrated with a model system and with realistic molecular calculations.

Exact Born-Oppenheimer decomposition of the many-body wavefunction for the complete system of electrons and nuclei.

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Abstract

We propose a new set of equations to treat non-adiabatic couplings between electrons and nuclei in molecular systems. The key idea behind the equations is to rewrite the many-body wave-function as a Born-Oppenheimer-type product of the nuclear $X(R, t)$, and electronic $\Phi_R(r, t)$, wave function. From the variational principle, we deduce formally exact equations for $X(R, t)$ and $\Phi_R(r, t)$. These represent the time-dependent generalization of already existing static equations (N.I Gidopoulos and E.K.U. Gross, cond-mat/0502433). These equations suggest time-dependent potential energy surfaces and a time-dependent Berry phase as rigorous concepts. These concepts will be illustrated by simple examples.

0.1.3 Posters

Ab-initio self-energy correction in systems with metallic screening

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Abstract

The calculation of GW corrections of the band structure for metallic systems shows the importance of considering the intraband contribution in the evaluation of the polarizability in its small- \mathbf{q} limit. When treated incorrectly, as in standard GW codes for semiconductor and insulators, it induces the opening of a spurious gap at the Fermi energy. A direct implementation for intraband contribution would require a Fermi-surface integration. To avoid this numerical overload we propose an approach based on determining the limiting behaviour of the polarizability by a fit of its Taylor expansion in the region where \mathbf{q} is small but finite. We test this method in the jellium case, and in the cases of Na and Al. Based on this adjusted polarizability we calculate the GW corrections for these systems, finding the expected bandwidth reduction (increase of the effective mass) with respect to the DFT bands, and of course no spurious gap.

Dielectric Function and Dielectric Matrix for Finite Momentum Transfer - Answers and Open Questions

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Abstract

Both the EEL spectrum and the dynamic structure factor as measured in inelastic x-ray scattering (IXS) are given by the imaginary part of the inverse dielectric function. Our combined experimental and theoretical work [1] of IXS and *ab initio* calculations carried out on silicon at different levels of approximation shows that time-dependent density-functional theory in adiabatic local-density approximation describes both the loss function *and* the dielectric function for non-zero momentum transfer very well for valence excitations in semi-conductors. The remaining differences are shown to be mainly lifetime related. We have also demonstrated the importance of crystal local-field effects and of the coupling between resonant and anti-resonant contributions to the imaginary part of the dielectric function. For sodium, on the other hand, the TDLDA fares much less well.

In our present poster we discuss several open questions which have to be solved in order to obtain a coherent and precise description of the response functions. This includes the off-diagonal elements of the inverse dielectric matrix which represent the local-field effects. Moreover, we discuss the influence of the pseudopotential description on the theoretical results. In particular, we will focus on the absorption edges which represent the contributions of the (semi-) core states. The influence of the core polarization on the spectra will be addressed as well.

[1] H.-Ch. Weissker *et al.*, PRL **97**, 237602 (2006).

Reflectance Anisotropy Spectroscopy study of ethylene on Si(001)

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Abstract

With the increasing demand for new organic devices compatible with current micro-electronics, the knowledge of the interaction of unsaturated hydrocarbon molecules such as ethylene, acetylene or benzene with silicon surfaces, is of particular interest. In spite of the large amount of experimental and theoretical works devoted to the study of the adsorption of ethylene, the simplest molecule containing a C-C double bond, on Si(001), some aspects of this process, such as the saturation coverage, or the adsorption geometry as a function of coverage, are still unclear. Here we study the interaction between C₂H₄ and a vicinal Silicon (001) surface by means of Reflectance Anisotropy Spectroscopy and analyze it with *first principles* calculations. Our results confirm that ethylene adsorbs without breaking the silicon dimers. Comparison of theoretical optical spectra with experimental data shows that the C₂H₄ molecules lay on top of the silicon dimers from low to high coverage. This occurs even though, from a purely energetic point of view, a bridge configuration would be favorite at saturation coverage.

Efficient ab-initio calculations of bound and continuum excitons

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Abstract

We present a scheme that yields different approximations for the exchange-correlation kernel of time-dependent density-functional theory (TDDFT). A specific choice of the approximation leads to the kernel that has been recently derived through the comparison with the Bethe-Salpeter equation [?, ?]. Another choice of the approximations leads to a static formulation of the kernel. We have checked the validity of this static approximation for a variety of materials such as Si, SiC, C and Ar. In all cases it is able to well reproduce the excitonic effects in the absorption spectra of these materials. Moreover the simplest static approximation yields a significant improvement of the scaling of the calculation with the size of the system.

Spin Polarisation and Electron Localisation in a Low-Density Electron Wire, A Density Functional Study.

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Abstract

Low-dimensional, high-mobility electron systems can be prepared by doping or laser irradiation of artificial semiconducting structures. Then, low electron density and low dimensionality stabilise spontaneous spin polarisation and electron localisation, which, in turn, may greatly affect the potential applications of these systems.

We investigate these phenomena by density functional (DF) computations for an idealised cylindrical jellium wire, using the local density approximation for exchange and correlation.

We employ a fully 3D representation of the system, and we determine the electron density and Kohn-Sham orbitals by direct energy minimisation in a plane wave basis.

Spontaneous spin polarisation and electron localisation arise at a density far above the values found in other DF studies, relying on radial and translational symmetry to simplify the computational task.

We present results for the charge and spin density exemplifying the variety of ground state configurations found in our study as a function of the jellium parameter r_s , the wire radius, and the net spin component (S_z) along the quantisation direction. We focus on systems at the boundary between different regimes, where solutions are found displaying a sizable amount of space and/or spin disorder, pointing to the stability of glassy low density configurations.

Although our results are certainly affected by the underlying local density approximation, we expect the global picture to remain valid in general, and to be relevant for experimental systems.

The dynamical structure factor from TDLDA - a tool to determine differences in the short-range structure in Si-high pressure phases?

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Abstract

Time-dependent-density-functional theory (TDDFT) within the adiabatic local density approximation (ALDA) is successfully employed to calculate the dynamical structure factor $S(\mathbf{q}, \omega)$ nowadays. Good agreement with experimental data obtained from inelastic x-ray scattering have been reported for different materials such as silicon [1], aluminum [2] or transition metal oxides [3].

In this work we explore the potential of TDLDA calculations of $S(\mathbf{q}, \omega)$ to detect changes in the local geometry of a material by performing calculations of three high pressure phases of Si, namely the β -tin, the primitive hexagonal and the hcp phase. These phases are particularly suited as they exhibit very distinct coordinations in their first neighbour shell. Our first results of calculations within the random-phase approximation (RPA) with and without local field effects at various values of \mathbf{q} show that local field effects only play a minor role in the excitation spectra. On the other side, including the TDLDA kernel leads to significant changes of the spectra with respect to the RPA results. Above all, at absolute q-values larger than ≈ 0.6 a.u. the spectra of the three phases differ significantly from each other. These differences can be attributed to the changes in the local coordination. Furthermore the differences in the excitation spectra are most pronounced if the direction of \mathbf{q} corresponds to the direction of the bonds in real space. Hence our results show that the dynamical structure factor calculated within TDLDA yields a fingerprint of the local structural properties in the different investigated phases of silicon. In the future we intend to compare our results with experimental data and apply this method to more complex systems.

[1] H.-C. Weissker, J. Serrano, S. Huotari, F. Bruneval, F. Sottile, G. Monaco, M. Krisch, V. Olevano, and L. Reining, *Phys Rev. Lett.* **97**, 237602 (2006)

[2] N. Maddocks R.W. Godby and R.J. Needs, *Europhys. Lett.* **27**, 681 (1994)

[3] I. G. Gurtubay, Wei Ku, J. M. Pitarke, A. G. Eguluz, B. C. Larson, J. Tischler and P. Zschack, *Phys Rev B*, **70**, 201201 (2005)

Ab initio optical absorption spectra of native and size-expanded xDNA base assemblies.

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Abstract

We present the results of time-dependent Density Functional Theory calculations of the optical absorption spectra of synthetic nucleobases and of their hydrogen-bonded and stacked base-pairs. We focus on size-expanded analogs of the natural nucleobases obtained through the insertion of a benzene ring bonded to the planar heterocycles (x-bases), according to the protocol designed and realized by the group of Eric Kool (e.g., Gao, J.; Liu, H.; Kool, E.T. *Angew. Chem. Int. Ed.* **2005**, 44, 3118-3122, and references therein). We find that the modifications of the frontier electron orbitals with respect to natural bases, which are induced by the presence of the aromatic ring, also affect the optical response. In particular, the absorption onset is pinned by the benzene component of the HOMO of each x-base (xA, xG, xT, xC). In addition, the main trait of the H-bonding inter-base coupling is a conspicuous red-shift of spectral peaks in the low-energy range. Finally, the hypochromicity, a well known fingerprint of stacking, is more pronounced in stacked xG-C and xA-T pairs than in stacked G-C and A-T pairs (also presented here), index of enhanced stacking.

Optical Spectra of Si Nanocrystallites: Bethe-Salpeter and Time-Dependent Density-Functional Theory

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Abstract

We present the optical absorption spectra of Si nanocrystallites containing up to 41 Si atoms within a method based on many-body perturbation theory (MBPT) and a method based on time-dependent density-functional theory (TDDFT). The method within the MBPT combines the Green-function screened-Coulomb-potential method (GW) and the solution of the Bethe-Salpeter equations (BSE) for the polarization function. The method based on TDDFT is applied for two different exchange-correlation (XC) functionals, the local-density approximation functional and the hybrid Heyd-Scuseria-Ernzerhof functional (HSE) to generate the XC potential in a generalized Kohn-Sham equation. We compare the optical and quasiparticle gaps in different approximations and evaluate the effect of setting the screened Coulomb potential and the XC kernel to zero, respectively in the GWBSE and TDDFT approaches. We verify that the influence of the electron-hole attraction on the optical absorption spectra is more important in the GWBSE scheme than in the TDDFT schemes, at least for the two XC functionals studied. With an appropriate choice of the functional, the TDDFT approach can reproduce several features of the GWBSE spectra.

Spectra of triatomic systems calculated using factorization method

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Abstract

The accurate and efficient method developed by A. Bordoni and N. Manini¹ and successfully used for 1D potential of diatomic molecules (e.g. H₂), is now being extended triatomic species. The exact diagonalization of an algebraically calculated matrix based on powers of the Morse coordinate have several advantages. It includes anharmonicity from the beginning, can be applied to a rich class of potentials (also double minimums), is (substantially) free from approximations, gives exact results in the limit of infinite basis size and is computationally efficient due to the matrix sparseness.

We present benchmark calculations on HCN molecule. The increasing degree of freedoms in polyatomic systems leads to more intricate form of both kinetic and potential energy. The *ab initio* potential has been fitted on a series of powers of two different Morse coordinates. The kinetic term is constructed in internal coordinates and goes beyond the harmonic coupling anharmonic oscillator (HCAO) approach.

¹A. Bordoni, N. Manini, *I. J. Quant. Chem.*, **107**, 782–797 (2007)

Spin-wave excitations from time-dependent density-functional theory

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Abstract

Spin waves constitute an important class of low-energy excitations in magnetic solids with a characteristic material-specific dispersion and a direct relation to magnetization dynamics. Until now most theoretical studies are based on the Heisenberg model of localized spins or on the frozen-magnon method, but neither is applicable to investigate the dynamics of spin waves in metallic systems with itinerant electrons. As a possible solution, time-dependent density-functional theory gives access to the full frequency-dependent transverse spin susceptibility, from which the lifetimes of spin-wave excitations as well as related spectral information can be extracted. We develop a practical scheme to calculate spin-wave spectra from first principles within this framework and illustrate its performance by applications to prototype ferromagnetic transition metals. Our implementation uses the full-potential linearized augmented-plane-wave method, and dynamic exchange-correlation effects are in the first instance described by the adiabatic local-density approximation.

Electronic deexcitation in semiconductors: towards a complete *ab initio* approach

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Abstract

Today, ultrafast time-resolved spectroscopy is a powerful tool to study the dynamics of carrier relaxation in semiconductors and complex materials. This technique gives access to detailed information on the interaction processes between elementary excitations. However, theoretical description of these processes is still incomplete and is often based on adjustable parameters [1,2].

At excitation energies smaller than two times the gap energy, the dynamics of carrier relaxation is determined by their interaction with phonons. The excited electrons interact with short-wavelength phonons (intervalley scattering), with polar optical phonons (Fröhlich interaction), and with acoustical long-wavelength phonons. To interpret the experiments of time-resolved spectroscopy, it is necessary to know the relaxation rates related to each deexcitation mechanism.

The goal of this work in progress is to develop a general *ab initio* approach for all deexcitation processes related to electron-phonon interactions. An approach to electron interaction with short-wavelength (intervalley) phonons is already established [3-5]. Our approach, which is based on Density Functional Theory and Density Functional Perturbation Theory, provides electron relaxation rates in good agreement with experiment, and can yield electron-phonon coupling parameters for the Monte Carlo simulations of optical and transport properties of semiconductors. As a next step, we are considering electron interaction with long-wavelength phonons: Fröhlich interaction, which is the dominant deexcitation process at high temperatures and at low carrier excitation energies, and electron-acoustical long-wavelength phonon interaction.

[1] C. Jacoboni and L. Reggiani, *Rev. Mod. Phys.* **55** (1983) 645.

[2] J. Shah, B. Deveaud, T. C. Damen, W. T. Tsang, A. C. Gossard, P. Lugli, *Phys. Rev. Lett.* **59** (1987) 2222.

[3] J. Sjakste, V. Tyuterev, N. Vast, *Phys. Rev. B* **74** (2006) 235216.

[4] J. Sjakste, V. Tyuterev, N. Vast, *Applied Physics A* **86** (2007) 301.

[5] J. Sjakste, N. Vast, V. Tyuterev, 2007, accepted in *Journal of Luminescence*

Implementation of an All-Electron G_0W_0 Code Based on FP-(L)APW+lo

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Abstract

The GW approach, applied as a first order correction to the Kohn-Sham eigenvalues (G_0W_0), has become the method of choice for the determination of quasi-particle excitations in semiconductors and insulators, for a review see [1]. Most of the existing codes are based on the pseudopotential (PP) method, where only the pseudo-valence states are included in the calculation of the self energy. A few years ago, the first full-potential (FP) all-electron implementations appeared [2,3], showing significant differences with PP results. Nowadays, there is an emerging consensus that G_0W_0 bandgaps are slightly underestimated in weakly correlated systems, provided that core states are adequately treated. Improvements have been obtained by the recently proposed quasiparticle self-consistent GW method [4], extending the ability to obtain accurate predictions of excited state properties for moderately correlated materials. Even qualitative agreement with experiments has been obtained for some strongly correlated systems [5].

The FP-(L)APW+lo method provides currently the most reliable results within density-functional theory. We have developed our own all-electron G_0W_0 code, based on the Wien2k implementation of the FP-(L)APW+lo method. As a basis set for the expansion of non-local operators we use the mixed basis set proposed in Ref. [1], which allows the inclusion of core and semicore states on the same footing. We have also extended the linear tetrahedron method to the calculation of \mathbf{q} -dependent Brillouin zone integrations. The singularity of the dielectric function as $\mathbf{q} \rightarrow 0$ is treated using $\mathbf{k} \cdot \mathbf{p}$ perturbation theory to obtain the limit analytically. The frequency dependence of the polarization is calculated numerically, without the need for further approximations like the plasmon pole model. All these features make this the most accurate implementation of the G_0W_0 approximation to date.

In this poster, we show the computational details of this implementation. Through a set of tests on different materials we analyse the efficiency and precision of the code as a function of the various dimensioning parameters (i.e. number of \mathbf{k} -points, frequencies, etc).

[1] F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998).

[2] W. Ku and A. G. Eguiluz, Phys. Rev. Lett. **89**, 126401 (2002).

[3] T. Kotani and M. van Schilfgaarde, Solid State Commun. **121**, 461 (2002).

[4] S. Faleev, M. Van Schilfgaarde, and T. Kotani, Phys. Rev. Lett. **93**, 126406 (2004).

[5] M. Van Schilfgaarde, T. Kotani, and S. Faleev, Phys. Rev. Lett. **96**, 226402 (2006).

EELS in graphene and carbon nanotubes: Linear plasmon dispersion

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Abstract

The fundamental analogy between graphene and single walled carbon nanotubes (SWCNT) is studied for collective excitations. Using the DP-code [1], we calculated momentum resolved energy electron loss spectra (EELS) for isolated graphene in RPA. Despite its two dimensional character, we find a linear dispersion of the pi-plasmon for in-plane momentum transfer. The comparison with experiment reveals its strong resemblance with the dispersion in isolated, vertically aligned SWCNTs along the tube axis. Interwall interaction between tubes can be modeled by means of two layer graphene.

[1] www.dp-code.org

Defect Formation Energies without the Band Gap Problem: Combining DFT and GW for the Silicon Self-Interstitial

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Abstract

Density-functional theory (DFT) has contributed greatly to our current microscopic understanding of the physical and chemical properties of defects in solids. The standard local-density or generalized gradient approximation (LDA or GGA), however, suffer from certain intrinsic deficiencies, most notably the band gap problem (BGP), that limit their predictive power. For the example of the silicon self-interstitial (Si_I) in silicon we illustrate here that the BGP – the fact that the Kohn-Sham eigenvalue gap underestimates the quasiparticle gap – not only affects the reliable computation of defect levels, but in certain cases also that of formation energies. By combining LDA with quasiparticle energy calculations in the GW approximation we reason why and present a new way to calculate defect formation energies in solids.

In the neutral charge state the Si_I has several stable and metastable atomic configurations, in all of which two electrons occupy a defect level in the band gap that derives largely from conduction band states. The formation energies of all configurations, however, are underestimated by about 1.5 eV compared to diffusion Monte Carlo (DMC) calculations [1,2]. While this appears like a disproportionately large amount, it corresponds roughly to twice the band gap underestimation of silicon in the LDA (~ 0.6 eV). Recent DFT calculations employing a hybrid functional that yields an improved band gap for silicon and formation energies for the Si_I

in much better agreement with DMC [2] lend further support to our BGP hypothesis.

By considering the formation of the neutral state as addition of 2 electrons to the $2+$ state, the formation energy can be decomposed into the formation energy of the latter ($E_f(2+)$), plus 2 electron affinities and subsequent relaxation energies. $E_f(2+)$ and the relaxation energies are now free from the BGP and can be reliably computed in LDA [3]. For the electron affinities we instead employ the GW method, which has become the method of choice for calculating electron addition and removal energies in solids. With this combined approach the formation energy increases by 1.1 eV compared to the LDA, slightly less than twice the band gap increase in GW .

[1] W.-K. Leung, R. J. Needs, G. Rapagopal, S. Itoh, and S. Ihara, Phys. Rev. Lett. **83**, 2351 (1999).

[2] E. R. Batista *et al.*, Phys. Rev. B **74**, 121102(R) (2006).

[3] M. Hedström, A. Schindlmayr, G. Schwarz, and M. Scheffler, Phys. Rev. Lett. **97**, 226401 (2006).

Fast polarizability and spin related stuff

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Abstract

Polarizability is a key ingredient for ab initio calculations in the framework of the Time Dependent Density Functional Theory. We show a quantitative analysis of the performances of an Hilbert transform based approach in speeding up the calculations of this quantity. We conclude that the method is particularly advantageous for systems presenting strong anisotropies for which the crystal local-field effects are important and the inclusion of the off diagonal terms in the GG'-matrix become not negligible. Moreover, according to the recent interest and trend on spintronic we implemented the spin degree of freedom in the DP code (www.dp-code.org) in order to be able to describe and predict spin related effects of materials. We are proceeding according to different steps of complexity and we present here some preliminary analysis of the response of simple systems in the collinear formalism.

Optimal Control of Two-Dimensional Nanodevices

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Abstract

We present a scheme to completely control single-electron quantum rings [1] and double quantum dots [2] by terahertz laser pulses. Our approach is developed in the framework of quantum optimal control theory (OCT) [3]. The theory yields, in principle, a laser pulse to drive the system from any initial state to any pre-defined target state. We show that when applied to rings and double dots, the optimized pulses generate the desired transitions in significantly shorter times and higher accuracies than previously used finite-length continuous waves. In quantum rings the controlled current-carrying states can be used to manipulate a two-level subsystem at the ring center, opening a path into a coherent single-gate qubit that has switching times of a few picoseconds. In double quantum dots our OCT approach enables a fast and controlled single-electron transport which, in contrast with the use of continuous waves, is insensitive to the dot geometry. In both systems the optimal pulse lengths are below the typical relaxation and decoherence times, which is promising for applications in quantum computing. The required terahertz frequency regime is routinely reached by, e.g., quantum cascade lasers, and the technology of pulse refinement is under rapid development [4].

[1] E. Räsänen, A. Castro, J. Werschnik, A. Rubio, and E.K.U. Gross, *Phys. Rev. Lett.* 98, 157404 (2007).

[2] E. Räsänen, A. Castro, J. Werschnik, A. Rubio, and E.K.U. Gross, <http://arxiv.org/abs/0707.0179>.

[3] A.P. Peirce, M.A. Dahleh, and H. Rabitz, *Phys. Rev. A* 37, 4950 (1988); R. Kosloff, S.A. Rice, P. Gaspard, S. Tersigni, and D.J. Tannor, *Chem. Phys.* 139, 201 (1989).

[4] M. Tonouchi, *Nature Photonics* 1, 97 (2007).

Numeric Atom-Centered Orbitals for Parallel and Scalable DFT in Periodic

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Abstract

We present the concepts of our new full potential, all electron local-orbital based electronic structure code, FHI-aims (“ab initio molecular simulations”) [1], with special emphasis on periodic systems. FHI-aims uses numeric atom-centered orbitals (NAO’s) $u_k(r)Y_{lm}(\Omega)$ as basis functions. Due to the flexible shape of the radial functions $u_k(r)$, small efficient basis sets can be constructed by adding only a few specific functions, yet with an accuracy comparable to other state-of-the-art methods (e.g. the full potential, linear augment plane wave (FP-LAPW) method) and the efficiency of plane-wave pseudopotential methods in large scale calculations. We demonstrate the accuracy of the method for surface energies of Au and Pt, in particular Au(100), which shows a quasihexagonal “5x20” reconstruction in experiment. For periodic systems the primary challenge with numeric atom-centered orbitals is the significant overlap of basis functions from different unit cells, leading to many (\mathbf{k} dependent) Hamiltonian and overlap matrix elements to be integrated and stored even in small unit cells. We minimize this integration effort by evaluating only those parts of all integrals that lie within one unit cell, employing sparse matrix storage in the process. All matrices are then constructed from these pieces in a separate step. Together with a density-matrix based charge density update and an electrostatic potential constructed from intermediate, finite analytical multipoles and a long-range Ewald sum [2], we demonstrate $O(N)$ -like scaling of all grid-based techniques in our approach for the large-scale 5x20 reconstruction of Au(100).

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, X. Ren, and M. Scheffler, *The FHI Ab Initio Molecular Simulations (aims) project*, Berlin (2007). [2] B. Delley, *J. Phys. Chem.* **100**, 6107 (1996).

Ab-initio calculation of electronic and optical properties of ZnO

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Abstract

ZnO is a widely studied material for its applications for spintronics, piezoelectric devices, chemical sensors and optoelectronics. The latter are favored by an exciton binding energy of 60 meV, which, being larger than room temperature thermal energy (26 meV), allows efficient excitonic emission without the need of cooling devices. ZnO-based room temperature polariton lasers can also be realized [1]. Finally, the possibility of tailoring its interesting properties exploiting quantum-size effects makes ZnO a very promising material for nanostructures [2]. From the theoretical point of view, ZnO is also challenging because of the difficulty of a proper treatment of semicore Zn 3d electrons. In this work, we study the electronic structure of wurtzite and zincblende ZnO, including quasiparticle effects in the GW approximation. It is shown how the choice of the number of electrons to be considered as valence in Zn pseudopotential affects the resulting electronic band structure. We then present calculated optical spectra, both for zincblende and wurtzite phases of ZnO, including excitonic effects through the solution of the Bethe-Salpeter equation. These results are compared with the ones obtained when excitonic effects are taken into account in an approximate fashion using the so-called $\hat{R}ORO$ kernel[3], which keeps into account the long-range Coulomb tail of the exchange-correlation kernel of TDDFT.

[1] M. Zamfirescu, A. Kavokin, B. Gil, G. Malpuech, and M. Kaliteevski, Phys. Rev. B 65, 161205 (2002).

[2] Z.R. Tian, J.A. Voigt, J. Liu, B. McKenzie, M.J. McDermott, M.A. Rodriguez, H. Konishi and H. Xu, Nat. Materials, 2, 821 (2003).

[3] L. Reining, V. Olevano, A. Rubio, and G. Onida, Phys. Rev. Lett. 88, 066404 (2002).

Quasiparticle calculations in α -SiO₂

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Abstract

We present results for the quasiparticle energies of α -SiO₂ obtained within the GW approximation using the LDA band structure as starting point. An efficient algorithm based on the spectral representation of the polarizability is employed to describe the dynamical dependency of the screened interaction $W(\omega)$. The self-energy operator $\Sigma(\omega)$ is numerically evaluated using two different techniques: the contour deformation method and an analytic continuation from the imaginary axis to the real axis. Alternatively, one can approximate $W(\omega)$ through plasmon-pole models. We compare the results for the optical gap and the quasiparticle corrections calculated from both the fully frequency-dependent method and the plasmon-pole approximation.

Quasiparticle calculations of band offsets of SiO₂ and ZrSiO₄ with Si

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Abstract

The size reduction of MOS transistor requires the usage of high-dielectric materials to replace SiO₂ as gate oxide layers. As the high- k /Si interface is formed, it is crucial that the band offsets be large enough to prevent electron or hole injection. In this study we have used first-principle DFT calculations within the local density approximation to study the band offsets of SiO₂/Si and ZrSiO₄/Si. We have included many body corrections as calculated by GW approximation. Indeed we have examined the capability of the quasiparticle corrections to predict the band offsets for a well known system as SiO₂/Si. The calculated band discontinuities were found to be in a good agreement with the experimental results.

Combining many body techniques with QM/MM for the calculation of optical properties of large scale systems: an application to indole in water solution

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Abstract

We develop a method to compute with high precision the optical properties of large scale systems. Realistic systems, especially in chemical and biological fields, are too large to be treated entirely by quantum calculations, but at the same time cannot be treated totally by a classical model because the physical phenomena studied involve electronic charge redistribution or electronic energy transitions like for example in the case of a chemical reaction or of an optical spectrum. Fortunately in many of these systems only a small part of the molecule needs to be treated by quantum calculations; in chemical reactions this part coincides with the active site of a compound. In this work we use this method to study optical properties of a solution. The DFT eigenvalues and eigenvectors are calculated by QM/MM and are used to solve GW and Bethe-Salpeter equations. We apply this new scheme to the study of indole in water and in vapor phase. The optical spectrum obtained considering the solvent as 'classical' is compared with those obtained introducing explicitly water molecules. Solvent shift, the number of snapshots needed and the effect of water on the electronic and optical properties of indole are discussed.

Theoretical spectroscopy for finite systems

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Abstract

This work deals with the calculation of linear-response properties of finite systems using time-dependent density-functional theory as well as many-body perturbation theory, namely GW and the Bethe-Salpeter equation. In particular we are interested in the performance of these methods when applied to large finite systems, e.g. biological systems. The existing theory we use for extended systems needs to be reformulated in order to make these calculations for large finite systems feasible. In this work we will discuss how we can obtain an efficient formulation for these systems.

Excitation energies in open-shell systems: facts, ideas, speculations...

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Abstract

The theoretical description of excited states of open-shell molecules is a difficult task, full of subtleties which are not always understood or made clear. We want to understand the failures of the present "state of the art" DFT- and MBPT -based methodologies, which cannot properly describe those excited states which have multiple-excitation character. It appears clear that these states would be described if the exact TDDFT kernel were used; however, when the adiabatic approximation to the exchange-correlation kernel is used, the calculated excitation energies have strict single-excitation character, and are fewer than the real ones. A frequency dependent kernel could create extra poles which would describe states with multiple excitation character [1]. The question is: how to introduce the correct ω -dependence in a general formulation? Maybe an answer can be obtained by starting from the Bethe-Salpeter equation, where a four-point kernel appears. Methods to derive a two-point kernel for TDDFT from the BSE kernel have been devised in the literature [2], and could be extended to the spin-polarized case.

[1] M. E. Casida, A. Ipatov, and F. Cordova, Linear-Response Time-Dependent Density-Functional Theory for Open-Shell Molecules, Lect. Notes Phys. 706, 243-257 (2006).

[2] F. Bruneval, F. Sottile, V. Olevano, R. del Sole, and L. Reining, Phys. Rev. Lett., 94, 186402, (2005).

Transport properties in nanotubes doped with DR1-Azobenzene

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Abstract

DR1-Azobenzene has two isomers. The most stable is the trans conformation, whose dipole moment is 9 D, while the cis conformation has a 6 D dipole moment. It is possible to pass from the trans- to cis-conformation (and vice versa) upon UV illumination. Recent experiments have demonstrated that DR1-Azobenzene can be physisorbed by nanotubes by means of anthracene, which acts as an anchor molecule. This physisorption produces changes in the transport properties of the nanotubes. In this way the transport properties of the nanotubes can be controlled through the isomerization process of DR1-Azobenzene with UV light. A crucial point to understand how the DR1-Azobenzene molecules affect the transport properties is to know their arrangement on the surface of the nanotube. In order to do this, we have built a model Hamiltonian which includes the interaction of anthracene with the nanotube surface and the dipole-dipole interaction among the DR1-molecules. The different parameters for this model Hamiltonian are obtained from BLYP calculations. Once the arrangement is known, we may evaluate the changes in the transport properties.

Towards an *ab initio* description of *f*-electron systems: an all-electron *GW* perspective

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Abstract

f-electron systems, i.e. materials containing atoms with incompletely filled *f*-shells, have received increased attention recently due to their diverse properties and wide range of applications. The physics and chemistry of these systems, however, remain largely elusive, because of the intricate nature of *f*-electrons and understanding them is regarded as one of the big challenges in condensed matter physics. In many materials the strong localization of the *f*-electrons competes with the coupling to itinerant electrons. valence electrons. The former gives rise to large many-body exchange and correlation effects, while the latter requires a quasiparticle description.

In these regimes density-functional theory in the local-density approximation (LDA) and its semi-local extensions is usually not adequate. Many-body perturbation theory in the *GW* approximation (GWA), however, offers a quasiparticle perspective and has become the method of choice for the description of quasiparticle band structures

in weakly correlated solids. Since exchange is treated at the exact-exchange level, the GWA appears to be a suitable method to identify those *f*-electron systems, in which the interactions are exchange dominated, and a natural starting point for methods that require a more sophisticated treatment of many-body interactions. So far applications of the GWA to *f*-electron systems are rare due to the high computational effort involved. We have developed an all-electron (AE) *GW* code based on the full-potential (linear) augmented plane wave (+ local orbital) method. As a first application to *f*-electron systems we have investigated cubic ZrO₂, HfO₂ and CeO₂. These materials have attracted growing interest in recent years as promising candidates for replacing SiO₂ as the gate dielectric in silicon-based field effect transistors. Moreover, CeO₂ plays an important role in catalysis. From a conceptual point of view they are interesting, because ZrO₂ has no *f*-electrons, CeO₂ an empty and HfO₂ a fully occupied *f*-shell. They therefore provide a good starting point for investigating the role of *f*-electrons. Our AE-GW calculations show that *f*-electrons have no effects on the quasiparticle corrections in HfO₂; the difference in electronic properties of ZrO₂ and HfO₂ are already well described at the LDA level. In CeO₂, the *f*-band falls in between the O 2*p* valence and Ce 5*d* conduction bands, and are therefore important at all levels of theory. We find that *GW* moves these bands into better agreement with experiment compared to the LDA.

The Role of Bound States in Time-Dependent Quantum Transport

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Abstract

We present a description of transport based on the time evolution of the non-interacting time-dependent Schrödinger equation and develop a numerical algorithm for the time propagation which is suited for implementation of time-dependent density functional theory. The algorithm is used to study time-dependent transport phenomena such as the role of bound state and transients in simple model systems. The presence of at least two bound states in the biased electrode-device-electrode system, leads to the current oscillations that remain undamped in the long-time limit. we also investigate the dependence of the TD-current on the history of applied bias, gate voltage and initial state.

Wave-vector-dependence Study of the Dielectric and Energy-loss Functions of small Carbon Nanotubes.

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Abstract

The anisotropic optical response of small-diameter single-walled carbon nanotubes is studied by means of ab initio calculations within the framework of the random-phase approximation. The dielectric and energy-loss functions are investigated for different non-zero momentum-transfer vectors. The importance of the inclusion of local field effects and plasmon dispersion are discussed.

Optical properties of 3-tert-butyl-cyclohexene from first principle methods

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Abstract

We are interested in the ab-initio description of the optical rotation of 3-tert-butyl-cyclohexene, a molecule composed of a cyclohexene ring C_6H_{10} and a butyl group $C(CH_3)_3$. For this molecule there is a discrepancy between experimental data and TDDFT (using local orbitals) results [1]. Our scope is to study the dichroism effects in this molecule within a plane-wave approach in order to explain this discrepancy. In a first step, we have studied the standard optical properties, meaning the dielectric function, for the two existing conformers a and b of this molecule within the independent particle approximation in DFT-LDA using a plane-wave expansion and within TDDFT using local orbitals. Preliminary results will be shown.

[1] D. M. McCann and P. J. Stephens, J. Org. Chem 71, 6074 (2006)

Efficient all-electron implementation of the GW approximation within the full-potential linearized augmented plane-wave method

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Abstract

The GW approximation for the electronic self-energy yields quasiparticle band structures in very good agreement with experiment, but almost all implementations so far are based on the pseudopotential plane-wave approach, which limits their range of applicability. We have developed an implementation within the full-potential linearized augmented plane-wave (FLAPW) method, which treats core and valence electrons on an equal footing. Furthermore, there is no artificial partitioning of core and valence densities. Within this method a large variety of materials can be treated, including d- and f-electron systems, oxides and magnetic systems. Our implementation employs a mixed basis set for the representation of basis-function products in the interstitial and muffin-tin regions. An expansion of the wave functions around $\mathbf{k} = \mathbf{0}$ using $\mathbf{k} \cdot \mathbf{p}$ perturbation theory allows us to treat the divergence of the Coulomb interaction analytically. The anisotropy of the dielectric screening is fully taken into account. A transformation of the mixed basis functions to the eigenfunctions of the Coulomb potential allows a reduction of the basis-set size without compromising the accuracy, which leads to a considerable speed-up in computation time. As a demonstration we show performance tests and results for selected solids.

Excitonic effects in semiconducting polymers - a comparison of TDDFT with the Bethe-Salpeter Equation

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Abstract

We perform first-principles calculations to study the optical properties of semiconducting polymers. Time-dependent density functional theory (TDDFT) on the one hand, and many-body perturbation theory (MBPT) on the other hand are employed to investigate the excitonic effects in the dielectric function. Both methods are implemented within an all-electron full-potential linearized augmented planewave (FPLAPW) scheme. The two semiconducting polymers, poly-acetylene (PA) and poly-para-phenylenevinylene (PPV), are discussed as examples for quite small (PA) and considerably larger (PPV) excitonic effects in the crystalline environment.

While the exciton binding energies are accessible through the solution of the Bethe-Salpeter Equation (BSE) within MBPT only, the excitonic spectra can be obtained within both theoretical approaches and compared to each other. Thereby, the BSE results provide a benchmark for the performance of the exchange-correlation (xc)-kernels within TDDFT. We show how sensitively the spectra behave with respect to the parameters of the semi-empirical long-range-kernels. Furthermore, we investigate whether a physical interpretation of these parameters is possible and what limits the applicability of this type of xc-kernels for these strongly anisotropic materials.

Time Dependent Density Functional Theory and Strongly Correlated Systems: Insight From Numerical Studies

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Abstract

We illustrate the potential of Time Dependent Density Functional Theory (TDDFT) for describing the nonequilibrium behavior of strongly correlated (lattice) models. Starting from an exact time-evolution of the many-body wavefunction, we determine, via reverse engineering, the exact exchange correlation (xc) potential v_{xc} for small Hubbard chains of different lengths and electron fillings and exposed to time-dependent perturbations. We compare some of the exact results to those of adiabatic-like treatments, in order to extract some of the properties that approximate xc potentials should have. Finally, we provide details of work in progress and future directions.

Mechanisms of photoinduced desorption in metal oxides

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Abstract

Recent experimental data clearly demonstrate that using both femto- and nano-second laser pulses with photon energies tuned to excite particular surface features at the MgO surface, one can achieve a very effective desorption of atomic O and Mg species. Moreover, new experiments show that emission spectra obtained on MgO nanocubes with maxima at 3.4 eV and 3.3 eV results from the excitation of 4-fold and 3-fold coordinated anions at 5.4 eV and 4.6 eV. In this presentation we demonstrate new mechanism responsible for desorption of Oxygen and Magnesium atoms and new mechanisms of photo-induced radiative and non-radiative processes on low-coordinated sites.

Recently we demonstrated that photo-induced desorption can be used for probing surface spectroscopic features [1-3]. The technique is sensitive enough to detect energy shifts between the bulk and surface excitons as small as 0.2 eV. In addition, a significant degree of control over the desorbed species can be achieved if the knowledge of the surface electronic structure is fully exploited [1-3]. We extended this approach to more complex oxide surfaces. The experimental and theoretical studies demonstrate that excitation energies of corner and step sites at the MgO (001) surface are strongly shifted with respect to the bulk and terrace exciton energies [4]. Recent experiments demonstrated that selective excitation of the kink and corner surface features using 4.7 eV laser pulses leads to desorption of O atoms with average kinetic energies of about 0.3 eV. Since the valence of anions in MgO is twice that of anions in alkali-halides, the desorption mechanism is expected to be more complex and involves several steps.

To model the photon-induced processes in MgO we employ an embedded cluster approach, which combines a quantum-mechanical treatment of a site of interest with a self-consistent classical description of the remaining part of the system. The method is implemented in a computer code GUESS; it allows one to account consistently for the ionic and electronic contributions to the defect-induced lattice polarization and for their effect on the defect itself, and to treat excited states using different ab initio techniques.

We modeled desorption from a 3-coordinated oxygen corner site at an MgO surface and developed a three-step mechanism for these processes [5-6]. The results of our calculations suggest that the first photon of ca. 4.5 eV can induce an optical transition at the oxygen corner site. This first excited state relaxes with a significant displacement of the corner oxygen away from its original site. The relaxed state corresponds to a charge transfer exciton configuration O... Mg⁺. This system can relax radiatively towards the ground state and the calculated value is 3.4 eV. However, calculations have shown also that nonradiative transitions to lowest triplet and ground state are allowed. If the system remains in the excited state, excitation with another photon at about 4.8 eV will ionise the corner (where the oxygen species has now a hole). Further photon at 4.8 eV excites the corner neutralizing the charge of Oxygen. The adiabatic potential energy surface for this excited state is such that oxygen atom prefers to leave the surface with the maximum kinetic energy of several tenths on an eV. The surface site relaxes with the formation of a F⁺ centre at the corner site previously occupied by the desorbed oxygen atom. Our results are in good agreement with the experimental photon energies and kinetic energies of desorbed species.

References:

- [1] V. E. Puchin, A. L. Shluger, N. Itoh, *Phys. Rev. B*, 47, 10760 (1993).
- [2] K. M. Beck, A. G. Joly, N. F. Dupuis, P. Perozzo, W. P. Hess, P. V. Sushko, A. L. Shluger, *J. Chem. Phys.*, 120, 2456 (2004).
- [3] W. P. Hess, A. G. Joly, K. M. Beck, P. V. Sushko, A. L. Shluger, *Surf. Sci.* 564 (2004).
- [4] A. L. Shluger, P. V. Sushko, L. N. Kantorovich, *Phys. Rev. B*, 59, 2417 (1999).
- [5] W. P. Hess, A. G. Joly, K. M. Beck, M. Henyk, P. V. Sushko, P. E. Trevisanutto, A. L. Shluger, *J. Phys. Chem. B*, 109 (42), 19563 (2005).
- [6] P. E. Trevisanutto, P. V. Sushko, A. L. Shluger, K. M. Beck, M. Henyk, A. G. Joly, W. P. Hess, *Surf. Sci.*, 593, 210 (2005).

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