

TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY: PROSPECTS AND APPLICATIONS

3rd International Workshop and School

Benasque (Spain), August 31 – September 15, 2008

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Supported by:



The third School and workshop was hosted by the Benasque Center for Science, located at the heart of the Pirinees. The aim of the school was to introduce theoretical, practical, and numerical aspects of Time-dependent-density functional theory (TDDFT) to young graduate students, post-docs and even older scientists that are envisaging a project for which TDDFT would be the tool of choice. During the school we incentivated a close and informal contact between the students and the teachers. Furthermore, the students presented their current research activities and future interests (two of those presentations were selected as oral contributions to the international workshop and were granted with the first Pedro Pascual Prize for the best posters of the school, see the enclosed document at the end of this report). We felt that this was an important point, since young scientists should be involved in the building up of a strong community. The number of applications (above 190) surpassed all expectations and, of course, the limit of 50 places that we had to satisfy in order for the students to get the maximum benefit from the school, and also due to space and computer resource limitations. The summary for the school is:

Sex	PhD students	Post-docs	Total
Female	9	3	12
Male	27	11	38

Moreover, the students (graduate and postgraduate) also did participate in the workshop held just after the 10 days of school. The total number of participants was 104 from all over the world (including 21 females; seven as invited speakers/lectures). The distribution between countries, experience and gender is provided in the following table:

	School	Teachers	Invited	Workshop	Total
Austria			1		1
Belgium	1				1
Brazil	3				3
Canada			1		1
Chile	1	1			2
Colombia	1				1
Czech Republic	1				1
Denmark	1				1
Finland	3		1	3	7
France	1	1			2
Germany	11	4	2	2	19
Greece			1		1
Iran	1				1
Ireland		1	1		2
Israel	1		1	1	3
Italy	8	6	4	3	21
Japan	1	2	1		4
Mexico	2				2
Netherlands	2	1		3	6
Poland	2				2
Portugal	2	3			5
Romania	1				1
South Korea	2				2
Spain	3	4			7
Sweden				1	1
Switzerland	1				1
Taiwan	1				1
UK		1			1
USA		1	3		4
TOTAL	50	25	16	13	104

The aim of the Workshop was to assess the present status of TDDFT approaches to the study of spectroscopic properties of real materials, and explore their capability for applications in further systems with technological and biological interest. The recent developments of TDDFT covered during the workshop include TDDFT versus current-DFT, van der Waals interactions, applications to biological systems, new functionals, transport phenomena, optical spectra of solids , etc. Due to the different

methods used to tackle this problem (Many-Body Theory, Density Functional Theory, Configuration Interaction, semi-empirical approaches), this Workshop was intended as a way to promote links among scientists coming from different communities working or interested in electron excited states. Also it was intended as a follow-up event for the students attending the school as it was a good opportunity for them to see the real implications of the school lectures and get the new theoretical advances in the the development of exchange-correlation functionals as well as applications to complex systems (nanostructures, bio-molecules, interstellar molecular analysis, solids, etc.) Our goal was to bring together scientists working on foundations and different applications of TDDFT and many-body theory, trying to assess the capability of current approximations to be applied to real systems of increasing complexity. The invited and contributed talks covered:

- I) Fundamental topics on TDDFT, Many-Body Theory, and electron transport theory.
- II) New approximations and techniques.
- III) Ab-initio calculations of spectroscopic properties of large scale systems.
- IV) Material Science, Nanoscience, Biology and Chemical applications.

As a consequence, there was a broad variety of participants which helped to get an interdisciplinary vision of the field. Thus, although some of the more specific topics were far from the research interest of many participants, the meeting was an excellent opportunity to see how the same techniques are used by members of other communities

School Program

<i>ay</i>	<i>Hour</i>	<i>Title</i>	<i>Theory/Practical</i>
(1) 1/9	9:30 - 10:15 10:30 - 11:15 11:30 - 12:15 12:30 - 13:15	TDDFT I (EG) TDDFT II (EG) Overview of spectroscopies I (MC) Many-Body: GW I (RG)	T
	15:00 - 18:30	Introduction to the practical classes	P
(2) 2/9	9:30 - 10:15 10:30 - 11:15 11:30 - 12:15 12:30 - 13:15	Overview of spectroscopies II (MC) TDDFT III (EG) Many-Body: GW II (RG) Theoretical spectroscopy (SB)	T
	15:00 - 18:30	Quantum Dots I (Documentation ; Code)	P
(3) 3/9	9:30 - 10:15 10:30 - 11:15 11:30 - 12:15 12:30 - 13:15	TDDFT IV (EG) Overview of spectroscopies III (MC) Propagation schemes (AC) Linear response theory (SB)	T
	15:00 - 18:30	Quantum Dots II	P
(4) 4/9	9:30 - 10:15 10:30 - 11:15 11:30 - 12:15 12:30 - 13:15	Advanced TDDFT I (NM) Current DFT I (CU) Overview of spectroscopies IV (MC) TDDFT as a tool in chemistry I (IT)	T
	15:00 - 18:30	Quantum Dots III	P

Workshop Program

Time dependent Density-Functional Theory: Prospects and Applications

3rd International Workshop and School

2008, August 31 - September 15

Workshop Program

Day I: Thursday 11th

Chairperson: Angel Rubio

09h00 - 09h10 E.K.U. Gross /
Angel Rubio Opening remarks

09h10 - 10h00 Kieron Burke Semiclassical origins of density functional theory

10h00 - 10h50 Roi Baer Dogmatic and Pragmatic Spirits in Time-Dependent Density
Functional Theory

10h50 - 11h20 Caffeine break

Chairperson: Neepa Maitra

11h20 - 12h10 Marc Casida TDDFT pushing the limits of and going beyond the adiabatic
approximation

12h10 - 13h00 Stephan Kuemmel Memory effects in real time: Probing the adiabatic
approximation in TDDFT

13h00 - 15h00 Lunch break

Chairperson: E.K.U. Gross

15h00 - 15h50 Andreas Goerling TDDFT with frequency-dependent exchange-correlation kernels

15h50 - 16h40 Kerstin Hummer Absorption spectra from TDDFT: do hybrid functionals account
for excitonic effects?

16h40 - 17h10 Beer break

Chairperson: Carsten Ullrich

17h10 - 18h00 John Rehr Real-time Approaches for Optical and X-ray Spectra

18h00 - 18h50 Xavier Andrade From TDDFT to Molecular Dynamics

Day II: Friday 12th

Chairperson: Rex Godby

09h00 - 09h50 Sohrab Ismail-
Beigi Optical properties of GaN nanotubes from many-body GW-BSE
perturbation theory

09h50 - 10h40 Yasutami Takada The electron self-energy in the Green's-function approach:
Beyond the GW approximation

10h40 - 11h10 Caffeine break

Chairperson: Robert van Leeuwen

11h10 - 12h00 R.W. Godby Exchange and correlation in quantum transport

12h00 - 12h50 Massimiliano di
Ventra Stochastic TDCDFT: a functional theory of open quantum
systems

13h00 - 15h00 Lunch break

Abstracts

School Poster Session

Electronic structure of topologically modified graphene sheets

Joice Araújo

UFMG - Universidade Federal de Minas Gerais

In this work, we address the electronic structure of graphene sheets modified by the addition of various different concentrations of heptagons and pentagons. An adjacent heptagon-pentagon pair (HPP), also known as a Stone-Waller defect, is a common defect in graphene and graphene-derived carbon forms such as nanotubes and fullerenes. An HPP is formed when a bond in the honeycomb network of graphene is rotated by 90°. Previously, Crespi et al. [1] have considered the electronic properties of planar graphene geometry in which all the hexagons were replaced by HPP's. The structure was shown to behave as a covalent metal, with a non-zero density of states at the Fermi level. In the present work, we consider graphene sheets consisting of dissociated HPP's. The dissociation of HPP's leads to the possibility of both planar and corrugated geometries, the latter being a result of non-null local curvatures at the heptagons and pentagons. We find the corrugated geometries to be more stable than the planar ones, and address the electronic structure of both varieties. We find that graphene sheets consisting of dissociated HPP's could behave as a metal, a semiconductor, or a semimetal, depending on the concentration of HPP's. We also address the electronic structure and energetics of grain-boundaries in graphene, as observed in a recent scanning tunneling microscopy study [2]. The grain boundary (GB) geometry is formed by HPP units along the GB line. We investigate the main electronic and elastic-energy features of GB's in this material as a function of the tilt angle.

[1] Vincent H. Crespi et al, Physical Review B 53, p. 303-305, (1996).

[2] P. Simonis et al; Surface Science 511, p. 319-322 (2002).

Computations on Metal-Phthalocyanines

Jakub Baran

Tyndall National Institute, University College Cork, Computational Modelling Group

Deposited and/or self-assembled on metal electrodes, metal-phthalocyanine are attractive candidates for novel molecular sensors, memory, and light-harvesting components. The knowledge of their molecular geometry and electronic structure are crucial points in order to understand their interactions with surfaces. To study the adsorption of metal-phthalocyanines (MPc (M=Co, Sn, Pb) bonded parallel on the Ag(111) surface we have performed electronic structure calculations using a cluster representation (55 and 169 silver atoms) of the surface within the framework of density functional theory (DFT) [1]. Our calculations use the generalized gradient approximation (GGA) parameterization

by Perdew-Burke-Ernzerhof (PBE) for the exchange-correlation energy [2] and multipole accelerated resolution of identity method [3]. We have investigated bonding on three surface adsorption sites (hcp-hollow, fcc-hollow and on-top). For each of these systems we have found good agreement in binding geometries with experimental data obtained by normal incidence X-ray standing wave spectroscopy (NIXSW) [4,5]. Binding energies and geometries for all systems are given. We propose flat chemisorption of respective MPCs on Ag(111).

Absorption geometry and interfacial properties for CH₃SH self assembled on Cu(110)

Stefania D'Agostino, Letizia Chiodo, Fabio Della Sala, Roberto Cingolani and Rosaria Rinaldi

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With the aim to characterize the real nature of the S-Cu bond and to shed light on the interfacial electrostatics for a copper surface, an ab initio study has been carried out for CH₃SH self-assembled on a Cu(110) substrate [1]. Calculations have been performed in the framework of the Density Functional Theory using the Generalized Gradient Approximation (GGA) [2] and the plane-waves code PWSCF [3] with Ultrasoft Pseudopotentials [4]. Theoretical results suggest that the binding of the methanethiol to the substrate is rather weak and that the molecular structure is correspondingly almost unaffected by the adsorption on metal. Otherwise, when CH₃SH decomposes by deprotonation producing methanethiolate (CH₃S), stronger chemical bonds appear between sulfur of CH₃S-radical and the surface Cu atoms. Experimental results on structural properties for this system give no clear informations on the adsorption site [5,6]. Therefore for a p(2x2) and a c(2x2) CH₃S coverage, a preliminary structural analysis on the relaxed geometries for various adsorption configurations has been necessary to elucidate the electronic properties at the molecule-substrate interface. By studying the partial density of states (PDOS) and the electrons accumulation/depletion regions in the real space, a strong hybridization among p-orbitals of sulfur and d-states from the metal substrate was deduced. Work function variations of CH₃S/Cu(110) were also monitored when the coverage changes between 0 ML and 1 ML: theoretical results prove an evident non-linear decrease at increasing coverage and this effect can be explained by the negative dipole of the adsorbate together with the interdipole effects.

[1] S. D'Agostino, L. Chiodo, F. Della Sala, R. Cingolani, R. Rinaldi, *Phys. Rev. B* **75**, 195444 (2007).

[2] J. P. Perdew, K. Burke, and M. Ernzerhof. *Phys. Rev. Lett.* **77**, 3865 (1996).

[3] S. Baroni, A. Dal Corso, S. De Gironcoli, P. Giannozzi, <http://www.pwscf.org/> (2001).

[4] D. Vanderbilt, *Phys. Rev. B* **41**, 7892 (1990).

[5] A. F. Carley, P. R. Davies, R. V. Jones, K. R. Harikumar, M. Wyn Roberts, and C. J. Welsby, *Topics in Catalysis* **22**, 161 (2003).

[6] J. G. Lee and J. T. Yates, *J. Phys. Chem. B* **107**, 10540 (2003).

Interpretation of valence band and resonant photoemission in the multiple scattering approach

Fabiana Da Pieve

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Valence band photoemission and resonant photoemission are widely used spectroscopic techniques. In particular, energy and angle resolved ultraviolet photoemission is a powerful technique for mapping energy bands of solids, while resonant photoemission has often been exploited to study correlation effects. We have extended the real space multiple scattering approach with the aim of interpreting experimental diffraction patterns and energy spectra obtained from transition metals both in the UV and X-ray regime. The LMTO method has been used for the calculation of potentials in the atomic sphere approximation and the exchange correlation part was calculated in the LDA approximation. For valence band photoemission we show that: 1) the real space multiple scattering approach, based on a finite cluster method, reproduces the band structure of the systems under investigation, as well as heavier band structure calculation 2) a dual behaviour between itinerant and well localized electronic states is observed when analyzing the anisotropy of UV diffraction patterns from Cu(111) when the analysis is performed energy-resolved or energy integrated For resonant photoemission in TiO₂ we show that: 1) we can describe the dependence of the spectra on photon energies and we reproduce the Fano profile originating from the interference between the resonant and the direct emission process. 2) the study of diffraction patterns allows to obtain informations on the delocalization of defect states.

Semiconducting chains of gold and silver

Frederico Ramos Fioravante

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Nanowires (NWs) based on $4d$ and $5d$ metals are a topic of intense current interest in the physics of nanomaterials. Understanding the connection between transport and atomic structure [1], in the limit of the ultrathin monoatomic wires that have been produced experimentally [2], is crucial to the future manipulation of metallic wires and electric contacts in nanoscale electronic devices. In order to study this connection we present an investigation of the relation between the atomic structure, energetics, and the electronic structure of ultrathin nanowires. In the limit of low-atomic-density (small diameters) wires, we introduce a geometry for ultrathin Au and Ag wires that *ab initio* calculations indicate to be more stable than previously considered planar geometries for these systems, by about 0.1 eV per atom. This structure is insulating for both metals and for related Ag_{0.5}Au_{0.5} alloys, with gaps of 1.3 eV for Au, 0.8 eV for Ag, and varying between 0.1 eV and 1.9 eV for the alloys. The insulating nature of the geometry is not a result of Peierls instabilities, and is analyzed in terms of an interplay between geometric and electronic structure effects. We also address more compact nanowires with volumetric structures. We find that gapped structures, with competing formation energies, may occur even for gold and silver, with gaps of 0.02 eV and 0.12 eV for silver and 0.25 eV and 0.13 eV for gold. Generally, we find that hollow tube-like structures are preferred for gold, while filled dimerized structures are more stable in silver nanowires. Our calculations also suggest the possibility of a great variety of structures with formation energies differing by the room-temperature scale, with different

numbers of bands crossing the Fermi level. This would suggest that the interpretation of quantum-conductance measurements must reflect this variety of electronic behaviors for a possibly larger number of degenerate structures.

[1] D. Cheng, W. Y. Kim, S. K. Min, T. Nautiyal, and K. S. Kim, *Phys. Rev. Lett.* **96**, Art. No. 096104, 2006.

[2] J. Bettini, F. Sato, P. Z. Coura, S. O. Dantas, D. S. Galvão, and D. Ugarte, *Nature Nanotechnology* **1**, 182 (2006).

CdSe nanocrystals under pressure

Giorgia Fugallo

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CdSe is an interesting material because of its efficient room temperature electro-luminescence and nano-electric device applications. In particular CdSe nanocrystals exhibit a range of interesting properties that can be tuned with their size: from the colours they fluoresce with to the way they change structure under pressure. By using and adapting the metadynamics method, which is able to accelerate rare events and to explore the free energy surface of complex systems, we have simulated structural transformations in CdSe nanocrystals close to the transition pressure, without the need to overpressurize the systems typical of conventional constant pressure molecular dynamics. Results for CdSe nanocrystals of different sizes and shapes will be presented.

AUTOMATIZATION OF FITTING THE DFTB REPULSIVE ENERGY

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SCC-DFTB is an approximation to density functional theory (DFT), starting from a second order expansion of the DFT total energy [1]. The total energy of a system is described by two contributions: an electronic and a repulsive energy. The fitting procedure for developing accurate and transferable parameters for the repulsive part has been cumbersome in the past. Recently first attempts were made for automating such a fitting procedure [2]. We are developing techniques for automatically producing repulsive parameters, following two approaches: 1) using a genetic algorithm and 2) by solving a linear equation system. We present preliminary results of these parameters for hydrocarbons as well as for small systems containing oxygen and hydrogen.

[1] M. Elstner et al., *PRB* 58(11) pp. 7260-7268 (1998).

[2] J. Knaup et al., *JPCA* 111(26) pp. 5637-5641 (2007).

Nickel oxide: spin and exchange effects

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The issue at the origin of this work is the nature underlying the considerable gap (4.3 eV) of nickel oxide. The question is whether the spin or the exchange interaction could contribute to its formation, or if maybe both could explain it. NiO is historically the prototype of the so-called "strongly correlated materials". The problem of its correct theoretical description was raised by N.F. Mott, since the paramagnetic phase of NiO was badly described by "band theories". He stated that strong correlation (strong d-electrons localization and repulsion) causes gap opening (Hubbard insulator) and prevents a band structure description (independent electrons approximation). The DFT-LDA calculations show us that spin leads to an insulating Kohn-Sham structure, whereas without it the system is in a metallic configuration. This is a well known result in literature. When a HF calculation is performed without accounting for the spin, NiO is still predicted to be a metal, as the DOS is non-zero at the Fermi level. Nevertheless, the density of states is heavily modified and loses most of its weight around the Fermi level. Introducing the spin in LSDA produces an insulating structure with an energy gap of about 0.5 eV, and the subsequent Hartree-Fock calculation predicts an insulator as well, with a high energy gap of about 14 eV (Hartree-Fock is known to highly overestimate the gap).

Discontinuity of the dielectric function close to Bragg reflections: Graphite.

R. Hambach, C. Giorgetti, N. Hiraoka, Y. Q. Cai, F. Sottile, A. G. Marinopoulos, F. Bechstedt, and Lucia Reining

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As an example for layered materials, the loss function of graphite was studied for momentum transfers q beyond the first Brillouin zone. Surprisingly, near Bragg reflections, the spectra are highly dependent on very small changes in q , which reminds the non-analyticity of the loss function in the optical limit ($q \rightarrow 0$). The effect is investigated by means of first principle calculations within the random phase approximation and experimentally confirmed by inelastic x-ray spectroscopy measurements. We explain this discontinuity by means of crystal local field effects that become particularly important and cause a strong coupling between excitations at small and large momentum transfers.

Full-Potential Multiple Scattering Theory with Space-Filling Cells for bound and continuum states

Keisuke Hatada

Multiple scattering (MS) approach has been widely used to solve the Schrödinger equation (SE) (or the associated Lippmann-Schwinger equation) both for scattering and bound states with energy dependent complex exchange correlation potential. Most practical calculations have been done within the so called “Muffin-Tin (MT) approximation” using cells of spherical shape, inside which the potential is spherically averaged and constant in the interstitial region. However the MT approximation cannot properly describe a great number of physical systems, ranging from open lattices to molecular systems with substantial anisotropy (eg. systems of biological interest), to surfaces and interfaces.

The first practical attempt to go beyond MT approximation with arbitrary shaped potential was done by Williams. [1] However it was soon realized that the method presented convergence problems in the angular momentum (AM) expansion. [2] One of the difficulties was to solve SE for arbitrarily shaped potential cells.

The present approach instead expands in spherical harmonics the wave function rather than the shaped potential, so that the convergence problem is completely avoided and we can treat arbitrarily shaped potential without any approximation. Together with appropriate numerical techniques this approach is seen to overcome the historical problem completely. [3]

We have tested the present FP-MS scheme against the analytical solution of the absorption cross section for hydrogen-like atoms in the case of the Li^{2+} atom ($Z=3$) by partitioning the system into 15 cells and an outer sphere. We show applications of the method to the calculation of the absorption spectra of molecules, Se_2 and GeCl_4 , and crystalline systems, Si and SiO_2 . We obtained significant improvement over the MT approximation in all cases.

[1] A. R. Williams and J. van W. Morgan, *J. Phys. C: Solid State Phys.* 7 (1974) 37.

[2] Y. Wang et al., *Phys. Rev. B* 49 (1994) 5028.

[3] K. Hatada et al., *Phys. Rev. B* 76 (2007) 060102(R).

Second order harmonic generation in crystalline semiconductors

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A comprehensive understanding of the nonlinear optical properties of solids is crucial for the improvement of nonlinear materials and devices and provides an opportunity to search for new materials. However, the theoretical description of nonlinear effects in solids is a formidable task and important difficulties have delayed any accurate calculations for many years. In principle the optical response of a material depends strongly on local field effects and electron correlations and important advances have been made recently to account for these in the linear response using Time Dependent Density Functional Theory (TDDFT) [1]. We formulate a derivation for the calculation of the second-order susceptibility tensor for crystals of any symmetry within 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 several materials with zincblende structure.

[1] F. Sottile, V. Olevano et L. Reining, Phys. Rev. Lett. 91, 056402 (2003).

A relativistic optimized potential method for spin-polarized systems

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We present the first implementation of a **spin-polarized relativistic** optimized potential method (ROPM) for solids in the framework of spin-density functional theory. We have reformulated the ROPM in terms of Green's functions and sketch our subsequent implementation within the framework of the KKR multiple-scattering theory for solids. This method is an all electron approach. All quantities are expanded in a fully relativistic spin-angular representation; spin-orbit coupling is treated **non-perturbatively**. Core-core interactions are determined along the lines of the method presented in Ref. [1], core-valence (band states) and valence-valence interactions are expressed in terms of the relativistic multiple-scattering representation. We used exact exchange (EXX) as a first step towards a complete exchange correlation functional. Results for simple metals are discussed.

[1] D. Ködderitzsch, H. Ebert, E. Engel, Phys. Rev. **B77**, 045101 (2008)

DFT analysis of the structural, electronic, and spectral properties of zFP538 chromophore

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The yellow fluorescent protein zFP538 isolated from button polyp *Zoanthus* belongs to a family of GFP-like proteins. The unique ability to form chromophore in an auto-catalytic reaction makes the group an attractive tool in biotechnology considering for instance applications like monitoring gene expressions or localizing proteins in living cells. Although numerous studies of the photophysical properties of GFP homologues, up to date, little is known about the nature of zFP538. The structure of its chromophore is of special interests, as the excitation and emission maxima have been found right between those of GFP and DsRed. The recently proposed structure of zFP538 chromophore contains an additional heterocyclic ring with the C=N bond comparing to GFP. As a result of increased conjugation in the chromophore the red shifts in spectra are being observed.

The main purpose of this study was the investigation of the structural, electronic and spectral properties of the chromophore zFP538 using theoretical methods. Based on Density Functional Theory (DFT) different protonation states of cis and trans isomers of zFP538 chromophore have been studied. The employed calculations let to analyse the dependence of zFP538 properties on environmental changes. To predict electronic excitation bands Time Dependent DFT (TDDFT) method has been chosen. All results presented in this work are significant in understanding details of zFP535 chromophore nature, as well as, bring new insights into the spectral properties of GFP-like proteins.

Optical Properties of Silicon Nanoclusters

Olli Lehtonen and Dage Sundholm

Department of Chemistry, University of Helsinki, Finland

Light emitting silicon nanoclusters have been studied extensively during last years. However, the actual mechanism responsible for the strong optical activity of the nanoclusters has remained unsolved. The molecular structures and electronic excitation spectra of silicon nanoclusters up to $\text{Si}_{329}\text{H}_{196}$ have been studied using time-dependent density functional theory. The computed excitation energies are often in good agreement with the experimental observations, but the oscillator strengths of the transitions are usually significantly smaller than reported in experiments. We have also proposed new class of silicon nanoclusters with silane modified surfaces, which have both energies and oscillator strengths in accordance with experiments, as possible candidates for strongly luminescent silicon nanoclusters.

Time-dependent density functional theory in projector augmented wave method

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In recent years, the time-dependent density functional theory has become a popular tool for calculating excited state properties such as linear and non-linear optical response. We have implemented the time-dependent density functional theory (TDDFT) using the projector augmented wave (PAW) method into the electronic structure program GPAW. Two different approaches, linear response and time propagation, are available. The real-space PAW has several advantages for both ground state and time-dependent calculations: single convergence parameter (grid spacing), different boundary conditions, reduced number of grid points (compared to pseudopotentials), and efficient parallelization using domain decomposition. As an example, we show a direct comparison of the linear absorption spectrum of the benzene molecule obtained via the time-propagation after a delta pulse and via the linear response calculation. We also demonstrate the excellent parallel performance of the time-propagation approach.

Quantum transport with correlations in Kadanoff-Baym approach

Petri MYÖHÄNEN

University of Jyväskylä, Finland

We consider an interacting two-level system coupled to macroscopic non-interacting electron reservoirs (leads). We apply the theory of non-equilibrium Green's functions to study the transient properties of the system driven by time-dependent bias voltage in different many-body approximations. Concepts such as history dependence, correlations and memory effects are also studied and analyzed.

The Lieb-Oxford lower bound on the exchange-correlation energy of atoms, molecules, solids and model Hamiltonians

Mariana Odashima

Universidade de São Paulo, Brazil

Density-functional theory (DFT) is one of the most popular and reliable approaches to the electronic-structure of matter. In DFT, ever better exchange-correlation functionals are required for the ever more precise description of many-body effects on electronic structure. Important ingredients in the construction of improved functionals are universal constraints, obeyed by all possible systems. Here we investigate one such universal property on approximate density functionals, the Lieb-Oxford lower bound on the exchange-correlation energy [1]. In a recent study [2,3] we showed, via case studies of atoms, ions, molecules, solids, and some model Hamiltonians, that the presently accepted value of this lower bound can be substantially reduced, leading to a tighter bound. We also point that different classes of systems can be classified with respect to class-specific (but not fully universal) similar bounds. A substantial change in this bound will have consequences for the performance of modern exchange-correlation functionals. Connections with the construction of such functionals will be explored.

[1] E. H. Lieb and S. Oxford, *Int. J. Quantum Chem.* 19, 427 (1981).

[2] M. M. Odashima and K. Capelle, *J. Chem. Phys.* 127, 054106 (2007). [3] M. M. Odashima and K. Capelle, *Int. J. Quantum Chem.* (accepted).

Accelerating RI-MP2 quantum chemistry calculations with graphical processing units

Roberto Olivares-Amaya

Harvard University

We present an algorithm to accelerate quantum chemistry calculations taking advantage of the graphical processing units (GPUs) as co-processors using CUDA and CUBLAS. We implement a method to virtually expand the GPU's memory in the face of data intensive calculations. Finally we also present 1.X precision, a method that circumvents the GPU's current ability to only give single precision calculations.

Non-adiabatic dynamics from ab-initio excited state potential energy surfaces

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Center for Individual Nanoparticle Functionality (CINF), Department of Physics, Technical University of Denmark.

We have generalized the method of Δ SCF-DFT to include situations where the relevant excited state is a superposition of Kohn-Sham orbitals as is the case for adsorbates on metal surfaces. From these

surfaces we can extract non-adiabatic coupling parameters and calculate probabilities for hot substrate electrons to transfer energy to the adsorbate. We find that at the level of single electrons we always need to treat the adsorbate quantum mechanically while given a thermal distribution of hot electrons we can treat the adsorbate semiclassically at the picosecond timescale when $T > 1000$ K.

Hunting double excitations processes

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Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia (CNISM); Physics Department, Università degli Studi di Milano, I-20133 Milan, Italy; European Theoretical Spectroscopy Facility (ETSF)

The spectra of isolated systems is known to be described quite well by Casida's approach to Time-Dependent Density-Functional-Theory (TDDFT) for many closed shell systems, within the adiabatic approximation. On the other hand the same framework is known to perform quite poorly for open shell systems. The reason of this deficiency can be found in the failure of the adiabatic approximation in describing double excitations, that leads, therefore, to the break of the spin symmetries of the system [1]. One would encounter analogous deficiencies using the Bethe Salpeter (BSE) approach with a static kernel $W_{\text{RPA}}(\omega = 0)$. A solution to the problem is the use of dynamical kernels. This work aims to scrutinize the dynamical structure that the BSE kernel and/or the exchange correlation kernel of TDDFT should have in order to describe double excitations. Following the same line of previous works on the study of removal/addition of electrons [2] and of excited states of nuclei [3, 4], we obtain the Feynman diagrams which should be included in the kernel. We show some preliminary tests on model systems and we give some guidelines for future developments.

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Efficient $O(N^2)$ approach to solve the Bethe-Salpeter equation for excitonic bound states

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The accurate calculation and parameter-free prediction of optical spectra including excitonic effects is highly desirable for both fundamental and applied research. Excitonic effects can be treated in the framework of many-body perturbation theory by solving the Bethe-Salpeter equation (BSE), which can be recast in an eigenvalue problem for the electron-hole Hamiltonian \hat{H} .

Although for the computation of excitonic optical spectra in an extended frequency range efficient methods are available, the determination and analysis of individual exciton states (e.g. excitonic

bound states or dark excitons) still requires the diagonalization of the electron-hole Hamiltonian \hat{H} . We present a numerically efficient approach for the calculation of exciton states with quadratically scaling complexity, which significantly diminishes the computational costs compared to the commonly used cubically scaling direct-diagonalization schemes. The accuracy and performance of this approach is demonstrated by solving the BSE numerically for the Wannier-Mott two-band model in k space and the semiconductors MgO and InN. For the convergence with respect to the k-point sampling a general trend is identified, which can be used to extrapolate converged results for the binding energies of the lowest bound states.

Ab initio study of the mechanism of production of photosensitized singlet oxygen by means of phenalenone

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The first excited state of molecular oxygen, singlet oxygen, is a reactive species that can mediate the oxidative degradation of many molecules. For most practical purposes, singlet oxygen is conveniently generated in a photosensitizing process wherein a molecule absorbs light and transfers a fraction of the excitation energy to the triplet ground state of oxygen to form singlet molecular oxygen.

Phenalenone (also called perinaphthenone, PN, fig.1) is a universal reference for sensitization of singlet oxygen. It's soluble in a large variety of solvents and its quantum yield for singlet oxygen production, Φ_{Δ} , is close to unity in most of the solvents. PN is present as a pollutant in the environment, and it is the skeleton of a lot of secondary metabolites that plants create for defence against pathogens. Its photodynamic therapy is demonstrated.

PN possesses an π,π -conjugated carbonyl group that is the main responsible for its photophysical and photochemical properties. After initial absorption to the second singlet excited state, the main deactivation process leads the system to the triplet state through an intersystem crossing with a quantum yield close to unity. Whereas triplet $n\pi^*$ states undergo photochemical reactions such abstraction of hydrogen, triplets $\pi\pi^*$ states show very efficient energy transfer reactions such as energy transfer to molecular oxygen. Therefore, $\pi\pi^*$ depends on the quantum yield of intersystem crossing and the character and the relative energies of the lowest triplet states.

The purpose of this work is to know the energetics and character of the lowest excited states of PN and elucidate the reaction path that populates the triplet state responsible of the sensitization of molecular oxygen. With this aim we have performed high level ab initio calculations with the protocol CASSCF/MS-CASPT2 to characterize the potential energy surfaces of the lowest singlet and triplet excited states of PN. We have calculated the vertical spectrum of the ground state minimum, located the critical points and crossing points (singlet-triplet crossing points and conical intersections) of the lowest PES, compute minimum energy paths (MEP's) and calculate spin-orbit couplings when necessary.

Characterization of (BN)_n Cage Emission Band Gaps exploiting Massively Parallel Analytical TDDFT Gradients

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Time dependent density functional theory is a main stream method for studying excitations in molecules and clusters. Gradients of the excitation energy [1] are needed to study the potential energy surface of excited states effectively. To extend the capabilities of existing implementations we have implemented time dependent density functional theory gradients in a modified version of NWChem [2] targeting massively parallel computing platforms. The resulting implementation has been demonstrated to scale up to at least 1000 processors. As a demonstration of the potential of this implementation we studied the optical properties of Boron-Nitride clusters. Boron-Nitrides are members of a family of III-IV semi conductors which can exhibit lasing as well as light emission. Of particular interest are cage structures that can be formed. The structure-property relationships were characterised focussing on absorption band gap modification by size selection and defects [3]. Exploiting the new capabilities the work was extended to characterise the emission band gaps as well.

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Optical excitations of surface defects in realistic nanoscale silica cluster

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We will discuss our work on predicting the absorption and luminescence spectra of realistic nanoscale silica cluster using TD-DFT and CASPT2. Special attention will be paid to a class of charge transfer defects that seem to require hybrid density functionals with an elevated fraction of Hartree-Fock like exchange for a proper description.

Workshop Poster Session

Theoretical spectroscopy for finite systems

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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.

GPAW: Projector-augmented wave method on real-space grids

Jussi Enkovaara

CSC - Scientific Computing, Helsinki, Finland

We have developed a program package GPAW for density functional calculations using real-space grids together with the projector augmented wave method. Real-space description allows flexible boundary conditions, efficient multigrid algorithms, and efficient parallelization with domain decomposition, while projector-augmented wave method enables accurate calculations for the whole periodic table. We present some applications of the method and demonstrate its efficiency especially in large scale parallel calculations.

Time-dependent natural orbitals with a phase

Klaas Giesbertz

VU University, Amsterdam

Density matrix functional theory (DMFT) has proven to be quite successful in producing ground state energies of bond breaking systems. Recently a also excited state curves became accessible by writing down the time-dependent DMFT equations [1,2]. However, the adiabatic approximation does not coincide with the static response equations in an earlier publication by Pernal [3]. This incompatibility can be lifted by an explicit treatment of a phase factor of the natural orbitals (NOs), although they are traditionally not defined, since the NOs are defined to be the eigenfunctions of the one-body reduced

density matrix. An additional advantage is that the two-electron system can truly be treated exactly, i.e. all single, double, triplet excitations are reproduced by the response equations that include the phase of the NOs.

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Linear density response function within the time-dependent exact-exchange approximation

Maria Hellgren

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We have calculated the frequency-dependent exact exchange (EXX) kernel of time-dependent (TD) density functional theory employing our recently proposed computational method based on cubic splines. With this kernel we have calculated the linear density response function and obtained static polarizabilities, van der Waals coefficients and correlation energies for all spherical spin compensated atoms up to Argon. Some discrete excitation energies have also been calculated for Be and Ne. As might be expected, the results of the TDEXX approximation are close to those of TD Hartree-Fock theory. In addition, correlation energies obtained by integrating over the strength of the Coulomb interaction turn out to be highly accurate.

Excitation Energy Transfer from a TDDFT real-time propagation approach

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Excitation energy transfer is a key process in the light-harvesting mechanism initializing the energy-converting machinery of plants and photosynthetic bacteria. Understanding how energy is transferred from one molecule to another one is a prerequisite for the tailored design of organic materials that serve in applications such as light-emitting diodes and organic solar cells. The standard method to interpret experimental data of excitation energy transfer between two molecules separated by a distance R is the so-called Förster theory. This theory considers separated donor and acceptor molecules interacting via a Coulomb interaction that is approximated as a dipole-dipole coupling. One of this theory's characteristics is a R^{-6} -dependence of the energy transfer rate. The aim of our work is to describe excitation energy transfer in the framework of TDDFT with real-time propagation. This approach in principle allows to go beyond the approximations of the standard (Förster) theory. Therefore, the method can be a valuable tool to distinguish between Förster like and non-Förster like excitation energy transfer.

Self-interaction correction and the Optimized Effective Potential

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University of Bayreuth, Germany

Self-interaction is one of the most substantial problems in present-day density functional theory. A widely used approach to overcome this problem is the self-interaction correction (SIC) proposed by Perdew and Zunger. However, the thus given functional does not only depend on the orbitals explicitly, but it is also variant under unitary transformation of the orbitals. Here, we present a recently developed generalized version of the Optimized Effective Potential (OEP) equation which is able to deal with both problems in one go [1]. To exemplify our approach we present calculations on organic molecular semiconductors. For these pi-conjugated systems semilocal functionals have recently been shown to suffer from large self-interaction errors [2]. In addition, we investigate the influence of the self-interaction error on the polarizabilities of molecular chains [3].

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A density functional theory for symmetric radical cations from bonding to dissociation

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It is known for quite some time that approximate density functional (ADF) theories fail disastrously when describing the dissociative symmetric radical cations R_2^+ . Considering this dissociation limit, previous work has shown that Hartree-Fock (HF) theory favors the $[R^{+1}-R^0]$ charge distribution while DF approximations favor the $[R^{+0.5}-R^{+0.5}]$. Yet, general quantum mechanical principles indicate that both these (as well as all intermediate) average charge distributions are asymptotically energy degenerate. Thus HF and ADF theories mistakenly break the symmetry but in a contradicting way. In this letter we show how to construct system-dependent long-range corrected (LC) density functionals that can successfully treat this class of molecules, avoiding the spurious symmetry breaking. Examples and comparisons to experimental data is given for $R=H$, He and Ne and it is shown that the new LC theory improves considerably the theoretical description of the R_2^+ bond properties, the long range form of the asymptotic potential curve as well as the atomic polarizability. The broader impact of this finding is discussed as well and it is argued that the widespread semi-empirical approach which advocates treating the LC parameter as a system-independent parameter is in fact inappropriate under general circumstances.

Modeling the non-adiabatic vibrational excitation of HCl on Au(111)

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University of Liverpool

Understanding the mechanisms playing a role in energy transfer when gas atoms impinge on metal surfaces is essential to understanding processes such as sticking, diffusion and reactivity. In addition to the mechanical energy transfer between molecule and surface, molecular vibrations may interact directly with electron-hole pair excitations of the solid. Recent measurements of the vibrational excitation probability of HCl molecules incident on a Au(111) surface suggest that there is a change in excitation mechanism as a function of the surface temperature from an electronically adiabatic mechanism to one involving excitation of electron-hole pairs [1]. This observation raises the question of whether the non-adiabatic coupling really is strong enough to explain the transition. We study the coupling of the HCl vibrations to electron-hole pair excitations by calculating first the non-adiabatic vibrational damping rate of the internal stretch mode for the adsorbed HCl molecule on Au(111) using time-dependent density-functional theory in the quasi-static limit [2]. Only the electronically non-adiabatic vibrational excitation is considered. We focus on constrained HCl collision trajectories along the surface normal with fixed molecule orientation and surface site. The vibrational damping rate and potential energy of the HCl molecule are calculated as a function of distance from the surface. The probability of the $n = 0 \rightarrow 1$ vibrational excitation is obtained by solving the master equation for the vibrational population using the calculated rates. Preliminary results for a few selected trajectories show that the calculated vibrational excitation probabilities are one order of magnitude larger than the experimental ones, a finding providing strong support for the hypothesis that non-adiabatic mechanisms play an important role in vibrational excitation of an HCl molecule when it scatters from a metal surface.

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Double excitations in finite systems

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Time-dependent density-functional-theory (TDDFT) is widely used in the study of linear response properties of finite systems. However, there are difficulties in properly describing excited states which have double- and higher-excitation character, particularly important in molecules with open-shell ground-state. These states would be described if the exact TDDFT kernel were used; however, within the adiabatic approximation to the exchange-correlation (xc) kernel the calculated excitation energies have strict single-excitation character, and are fewer than the real ones. A frequency-dependent xc kernel could create extra poles in the response function, which would describe states with multiple-excitation character.

We introduce a frequency-dependent xc kernel which can reproduce, within TDDFT, double excitations in finite systems. In order to achieve this, we use the Bethe-Salpeter equation with a dynamical

screened Coulomb interaction $W(\omega)$ which can describe these excitations. We test this kernel on a two-electron model systems, and we find that poles corresponding to double excitations are produced. However, together with the expected energies, other poles corresponding to unphysical states appear. We attribute this deficiency to the self-screening problem the description of $W(\omega)$ suffers from.

Ultrafast manipulation of electron spins in a double quantum dot device: A real-time view

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We consider a double quantum dot system with two embedded and non-aligned spin impurities to manipulate the magnitude and polarization of the electron spin density. The device is attached to semi-infinite one-dimensional leads which are treated exactly. We provide a real-time description of the electron spin dynamics when a sequence of ultrafast voltage pulses acts on the device. The numerical simulations are carried out using a spin generalized and modified version of a recently proposed algorithm for the time propagation of open systems [Phys. Rev. B **72**, 035308 (2005)]. Time-dependent spin accumulations and spin currents are calculated during the entire operating regime which includes spin injection and read-out processes. The full knowledge of the electron dynamics allows us to engineer the transient responses and improve the device performance. An approximate rate equation for the electron spin is also derived and used to discuss the numerical results.

Contribution of electron-ion correlations to the non-adiabatic dynamics of conjugated oligomers

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London Centre for Nanotechnology and University College London

Non-adiabatic processes play a central role in energy transfer between electronic and ionic degrees of freedom in photoexcited conjugate polymers due to their strong electron-phonon coupling. In particular, we are interested in modelling the photogeneration of topological excitations — polarons and excitons — following an earlier vertical transition from the fully relaxed ground state to a low-lying dipole-allowed electronic level. A crucial quantity to study is the ratio between the number of charged and neutral excitations generated because the efficiency of many organic electronic devices strongly depends on it. Here we present the application of a numerical scheme based on Correlated Electron-Ion Dynamics (CEID) to a simple model of conjugated oligomers and we show that electron-ion correlations can effectively suppress the photogeneration of charged topological excitations (polarons) even when electron-electron correlations are not included. Our findings are in agreement with recent experiments and they can shed more light on the physics of organic electronic devices.

Time-dependent density-functional theory for electron-atom scattering

Meta Van Faassen

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We present a method to obtain single-channel elastic electron-atom scattering phase shifts from time-dependent density functional theory (TDDFT). The system is placed in a spherical box, and TDDFT is used to calculate its discrete spectrum, from which phase shifts are deduced. Results for scattering from different atoms are shown. We also show scattering results using a finite Slater type basis set (STOs), which simplifies implementation in existing bound-state DFT computer codes.

Workshop Invited Talks

Optical properties of GaN nanotubes from many-body GW-BSE perturbation theory

Sohrab Ismail-Beigi

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We present our recent work on the electronic, optical, and luminescent properties of single-walled gallium nitride nanotubes as predicted by the first principles many-body Green's function GW-Bethe Salpeter Equation (BSE) approach. Along the way, we also will review and discuss GW-BSE for such nanosystems from a pragmatic viewpoint: e.g. what does one do in typical GW-BSE calculations? How expensive are GW-BSE calculations for nanostructures? How do they scale? What physical, mathematical, and algorithmic issues can make GW-BSE expensive? And how can one overcome or circumvent some of the hurdles?

Dynamics in dielectrics induced by ultrashort laser pulses

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Laser spectroscopy techniques employing an ultrashort laser pulses are rapidly developing not only to measure optical properties of materials but also to control them. The optical electric field first excites electrons and then the excitation energy is transferred to the ions. We apply the real-time TDDFT to describe the electron-ion dynamics in dielectrics induced by the laser pulse.

When the strength of the electric field of laser pulse is comparable to the electric field which binds electrons in materials, a variety of phenomena reflecting nonlinear electron dynamics are observed. They include multiphoton and tunnel ionizations, rescattering phenomena which induce high harmonic generation in atoms and molecules, and optical breakdown in dielectric materials. In my presentation, I would like to discuss two topics, a description of the optical dielectric breakdown described by the time-dependent Kohn-Sham equation [1] and a description of coherent phonon in dielectrics.

Our basic equation to describe the electron-ion dynamics in periodic systems is the time-dependent Kohn-Sham equation for the Bloch function in which the induced polarization field as well as the external laser electric field are treated as the time-varying, spatially uniform vector potential [2]. The time-evolution of the induced vector potential is determined by the current averaged over the unit cell. The forces acting on ions are evaluated with the electron density distribution at each time step..

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Absorption spectra from TD-DFT: Do hybrid functionals account for excitonic effects?

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The accurate description of optical absorption spectra of extended systems is a long standing challenge to computational physics. The basic prerequisite for obtaining highly reliable excitation spectra, is the inclusion of many-body effects, in particular, the electron-hole interaction. Two state-of-the-art approaches for calculating electronic excitation spectra exist. These are (i) many-body perturbation theory commonly within the GW approximation combined with a subsequent solution of the Bethe-Salpeter equation (BSE) and (ii) time-dependent density functional theory (TD-DFT). Since the GW /BSE approach requires the technically cumbersome diagonalization of a two-particle matrix and the \vec{k} -point convergence of optical spectra is rather slow, such calculations are exceedingly time consuming and presently reported for systems containing up to 100 atoms only. In contrast, in the TD-DFT approach all many-body effects are taken into account by the frequency-dependent exchange correlation (xc) kernel $f_{xc}(\vec{r}, t, \vec{r}'; t')$, which, however, is not explicitly known for real systems. Approximations for f_{xc} based on the homogeneous electron gas (local functionals) lack any long-range interactions and thus fail to account for excitonic effects. Moreover, absorption spectra calculated using standard local or semi-local xc functionals are usually significantly red-shifted due to the well known underestimation of the band gaps. The latter shortcoming can be much improved by the application of hybrid density xc functionals, that mix a small amount (typically 25%) of the non-local Hartree-Fock exchange term to the semi-local functional. In particular, the recent suggestion of Heyd, Scuseria, and Ernzerhof of a screened exchange term (HSE functional) has enabled an efficient treatment of extended systems [1]. This functional yields impressive band gaps of many solids [2,3] and thus the question arises, whether it also improves the description of optical absorption spectra and related properties such as the static dielectric constants.

For the determination of the static and dynamic dielectric function, we first calculate the occupied and a few unoccupied one-electron states using the HSE functional and the plane wave PAW code VASP [4]. Instead of solving the Casida equation, which is the analog of the BSE equation for non-local hybrid functionals, we determine an effective non-local $f_{xc}(\vec{r}, \vec{r}')$ using the approach of Reining, Del Sole, and Marini *et al.* [5,6,7,8].

The main achievement of the present work is to show that the HSE functional substantially improves the description of the static and dynamic screening properties compared to standard semi-local functionals. This includes the correct prediction of the oscillator strength for low energy excitations. However, as opposed to the GW /BSE approach, absorption spectra are only reliable for systems with a medium band gap and a static dielectric constant $\epsilon \gtrsim 4$.

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TDDFT with frequency-dependent exchange-correlation kernels

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A new density-functional response method is introduced that is well-suited for the use of orbital-dependent exchange-correlation kernels. In particular, a new TDDFT approach employing the frequency-dependent exact exchange kernel is presented. The approach is implemented within a Gaussian basis set framework. Its general performance and its performance in treating charge transfer excitations is discussed. The relation of the approach to time-dependent Hartree-Fock is considered. General limitations of TDDFT methods in the response regime are pointed out.

Real-time Approaches for Optical and X-ray Spectra

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Real-time approaches are becoming increasingly important in understanding various photon spectroscopies ranging from linear and non-linear optical response to x-ray absorption spectra (XAS). Here we discuss two such real-time approaches.

I. The first is a real-time, time-dependent density functional theory (RT-TDDFT) approach for ab-initio calculations of frequency-dependent linear and non-linear optical response. This method is an extension to hyperpolarizabilities of an approach based on calculations of the time-evolution operator using the electronic structure program SIESTA. Instead of calculating excited quantum states, which can be a bottleneck in frequency-space calculations, the response of large molecular systems to time-varying electric fields is calculated in real-time. To speed the non-linear calculations, our approach uses Gaussian enveloped quasi-monochromatic external fields. With this approach we obtain frequency dependent second harmonic generation (SHG), the DC nonlinear rectification, and the electro-optic effect (EOE). The method is illustrated with calculations for nano-scale photonic nonlinear optical (NLO) molecules, and yields results in good agreement with experiment.

II. The second approach is based on real-time simulations of the dynamic structure of nano-scale materials based on finite-temperature density functional theory/molecular dynamics and x-ray spectroscopy theory. This approach is illustrated for the case of Pt nanoclusters supported on gamma-alumina using temperature-dependent. These simulations reveal a complex dynamical structure on multiple-time scales including a hindered Brownian-like librational motion of the center of mass and fluctuating bonding, and explain many of the unusual properties observed for such materials.

Electron Transfer and Electron Transport: Fighting Self-Interaction in TDDFT

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This talk will highlight ongoing work aimed at describing charge transfer processes accurately with existing functionals. In the first part, we will show how applying well-motivated constraints to the electron density allows one to describe charge transfer excited states on the same footing with the ground state. This principle will be illustrated for the case of simple organic photochemistry. In the second part of the talk, we will address the extension of these concepts to the case of electron transport through junctions. We will show numerically that a reasonable approximation to the steady state current can be obtained from a large but finite closed system calculation. By employing different approximations to exchange and correlation, we investigate the impact that different approximate functionals have on the transport process. Our results suggest that the impact of self-interaction is much more pervasive for dynamically open systems than it is for eigenstates.

Dogmatic and Pragmatic Spirits in Time-Dependent Density Functional Theory

Roi Baer

The Hebrew University of Jerusalem, Israel

Dogmatic spirit: prevalence of the adiabatic approximation in TDDFT.

Pragmatic spirit: adjustable range parameter for avoiding self-repulsion effects DFT and TDFDT.

TDDFT and Strongly Correlated Systems: Insight From Numerical Studies

Claudio Verdozzi

Lund University, Sweden

We illustrate the scope of Time Dependent Density Functional Theory (TDDFT) for strongly correlated (lattice) models out of equilibrium. Using the exact many body time evolution, we reverse engineer the exact exchange correlation (xc) potential v_{xc} for small Hubbard chains exposed to time-dependent fields. We introduce an adiabatic local density approximation (ALDA) to v_{xc} for the 1D Hubbard model and compare it to exact results, to gain insight about approximate xc potentials. We also provide some remarks on the v -representability for the 1D Hubbard model. Finally, we present some results from work in progress.

Structural and optical transitions of the Biliverdin chromophore

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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 recently 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 around the chromophore 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, the 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 infrared, Raman, and optical 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.

The electron self-energy in the Green's-function approach: Beyond the GW approximation

Yasutami Takada

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More than four decades ago, Hedin derived a set of exact relations among the one-electron Green's function G , the electron self-energy Σ , the effective electron-electron interaction W , the polarization function Π , and the vertex function Γ [1]. If Γ were set equal to unity, those relations could be solved self-consistently in an iterative way, leading to the so-called GW approximation. This approximation, however, violates the basic conservation law of the local electron number or the Ward's identity, necessitating the proper inclusion of Γ in determining Σ .

Starting from the Bethe-Salpeter equation for Γ with use of the proper irreducible electron-hole interaction as the integral kernel and an analogous equation for the current vertex function, I have derived a useful form for Γ as a functional of G or $\Gamma = \Gamma[G]$. This form, which is formally exact, is very convenient in constructing an accurate-enough approximation scheme for Γ . Then the *GWT* method can be defined by the insertion of such a scheme for $\Gamma[G]$ in the self-consistent iteration loop to determine Σ simultaneously with G , W , and Π .

In my talk, I shall (1) derive the useful and exact form for $\Gamma[G]$ in which I will introduce a few key physical quantities such as the one leading to a modified Lindhard polarization function, (2) point out various possible approximation schemes for $\Gamma[G]$ depending on the problems in hand, (3) explain a successful form for $\Gamma[G]$ in the uniform electron-gas system exploiting the concept of the local-field correction [2], (4) verify that (although the GW approximation fails) my result successfully reproduces the experimentally observed bandwidth of the Na 3s occupied states [3], and (5) discuss future prospects of this *GWT* method in comparison with a recent similar proposal [4].

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

[2] Y. Takada, Int. J. Mod. Phys. B 15, 2595 (2001).

[3] Y. Takada, Phys. Rev. Lett. 87, 226402 (2001).

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

Semiclassical origins of density functional theory

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I will explain how density functional theory works, and why different functionals are used for different purposes. This includes the origin of PBEsol, a variation on PBE for solids, and the best way to approach orbital-free DFT. I will discuss the time-dependent problem, if I have results.

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2008 Poster Prize Winners



PEDRO PASCUAL POSTER PRIZE

MR. PETRI MYÖHÄNEN HAS BEEN AWARDED EXEQUO WITH MR. INGOLL WARNKE THE 1ST PEDRO PASCUAL PRIZE FOR THE BEST POSTER PRESENTED DURING THE THIRD SUMMER SCHOOL POSTER "TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY: PROSPECTS AND APPLICATIONS" HELD IN BENASQUE FROM THE 31ST OF AUGUST TO THE 9TH OF SEPTEMBER.

BENASQUE 9TH SEPTEMBER 2008

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