European Science Foundation (ESF)
1 quai Lezay Marnesia
BP 90015
67080 Strasbourg Cedex
France

14th of January, 2010

Dear Dr. Chantal Durant,

I am writing to confirm that the quantity of 9600.00 Euros has been received by the CENTRO DE CIENCIAS DE BENASQUE “PEDRO PASCUAL”. Please find a detailed description of the expenses that amount to the sum of 12000 agreed from the project Simbioma. We look forward to receive the remaining 2400.00 Euros.

The money has been used as financial support to cover the registration fee, travel and accommodation expenses for students attending the school “Time-Dependent Density-Functional Theory” held in Benasque from the 2nd to the 15th of January, 2010.

Please find enclosed a table showing the distribution of funding amongst the students and lectures. Copies of the bills will be sent to you by surface mail as soon as possible.

Dr Angel Rubio, the scientific organiser of the school will send a detailed scientific report in due time.

Yours sincerely,

José Ignacio Latorre
Director

SimBioMa: Funding distribution

Surname	First name	Nationality	Daily Allowance	Travel support	Accommodation Support	Payment	Return	Amount received (euros)
ATTACCALITE	Claudio	Italian	336.60	202.29	361.50	0.00	0.39	900.00
AMBROSCH-DRAXL	Claudia	Austrian	187.00	276.20	436.80	0.00	0.00	900.00
DREIBIGACKER	Ingo	German	112.20	0.00	800.00	0.00	12.20	900.00
EPURE	Luiza	Romanian	411.40	0.00	503.10	0.00	14.50	900.00
FINN	James	British	187.00	89.00	624.00	0.00	0.00	900.00
GHANE	Tahereh	Iranian	523.60	71.40	305.00	0.00	0.00	900.00
GHOSH	Prasenjit	Indian	0.00	177.00	723.00	0.00	0.00	900.00
GOVONI	Marco	Italian	523.60	71.40	305.00	0.00	0.00	900.00
HUIX	Miquel	Spain	523.60	72.20	305.00	0.00	0.80	900.00
OLIVEIRA	Micael	Portuguese	411.40	127.10	361.50	0.00	0.00	900.00
MARTIN	Fernando	Spainish	112.20	209.00	140.00	138.80	0.00	600.00
NOGUEIRA	Fernando	Portuguese	598.40	429.40	472.50	0.00	0.30	1500.00
VARSANO	Daniele	Italian	336.60	191.00	289.00	83.40	0.00	900.00
							TOTAL	**12000.00** **Euros**

TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY: PROSPECTS AND APPLICATIONS

4th International Workshop and School

Benasque (Spain), January 2 – 15, 2010

A. Rubio (Univ. País Vasco and ETSF, Spain),
E. K. U. Gross (MPI Halle, Germany),
M. A. L. Marques (LPMCN, Université Lyon I, France),
F. Nogueira (CFC, Univ. de Coimbra, Portugal)

Supported by:

SPONSORED BY:
Marie Curie Series of Events program: Psi-k Training in Computational Nanoscience
European Theoretical Spectroscopy Facility
Lightnet Network of Excellence
ESF SimBioMa Programme
ESF IntelBioMat Programme
CECAM
Spanish Ministry of Science and Technology
Benasque Center for Science
Universities of the Basque Country and Coimbra

The fourth school and workshop was hosted, as the previous ones, by the Benasque Center for Science. The aim of the school was to introduce theoretical, practical, and numerical aspects of time-dependent-density functional theory (TDDFT) to young graduate students and post-docs interested in the tool in itself or planning to use it for their own research. The physical conditions offered by the new Benasque Center for Science (http://www.benasque.org/) allow for a very fruitful and informal contact between the students and the teachers, that we strongly encouraged.

All the pedagogical documents of the school are made available to the everybody through the webpage of the meeting (http://www.benasque.org/2009tddft/). Also, as in previous editions we provided all the students with the book "Time-Dependent Density-Functional Theory", edited by M.A.L. Marques, C. Ullrich, F. Nogueira, A. Rubio, and E.K.U. Gross, *Lecture Notes in Physics* (Springer: Berlin, 2006), as it has all the basic material to be discussed in the lectures. We plan to have a new edition of the book (completely revised based on the input of the students in the last schools) by the next event (5th school to be help in Benasque also in winter, january, 2012).

In order to allow for the students to better discuss their research projects among themselves and with the teachers of the school, we asked them to present posters describing their current work and/or planned research project. Two of these posters were then selected as oral contributions to the international workshop and were granted the second Pedro Pascual Prize for the best posters of the school. As in previous editions of this event, the number of applications (above 180, the largest of all the events organised till now) surpassed all expectations and, of course, also the limit of 48 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 participants in the school were distributed in the following way:

Sex	PhD students	Post-docs	Total
Female	9	2	11
Male	25	12	37

All the students participated also in the workshop held just after the 8 days of school. The total number of participants was 101, with 31 different nationalities from 5 continents. There were 21 female participants, six of them being invited speakers/lecturers. The distribution between countries, experience and gender is provided in the following table:

	School	Teachers	Invited	Workshop	Total
Argentina	1				1
Australia	1		1		2
Austria	1		1		2
Belgium	1	1			2
Canada			1		1
Chile		1			1
China	1				1
Colombia	1			1	2
Czech Republic	1				1
France	1		1	1	3
Germany	5	4	5	4	18
India	4				4
Iran	1			1	2
Ireland		1			1
Israel			2	1	3
Italy	7	6	2	2	17
Japan			1	1	2
Korea	1				1
Mexico	1				1
Morocco	1				1
New Zealand		1			1
Portugal	1	3	1		5
Romania	1				1
Russia	2	1	2		5
Spain	6	3	1	1	11
Sweden	1				1
Switzerland		1	1		2
Turkey	1				1
UK	4				4
Ukraine	1				1
USA	3				3
Male PhD	25	2		5	32
Female PhD	9			1	10
PhD	**34**	**2**		**6**	**42**
Male Post-doc	12	17	16	3	48
Female Post-doc	2	3	3	3	11
Post-doc	**14**	**20**	**19**	**6**	**59**
Male	37	19	16	8	80
Female	11	3	3	4	21
# Participants	**48**	**22**	**19**	**12**	**101**

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 systens.
IV) Materials 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

Day	**Hour**	**Title**	**T/P**
1 (3/1)	8h30 – 9h15	TDDFT I **(EG)**	T
	9h30 – 10h15	TDDFT II **(EG)**	T
	10h30 – 11h15	Overview of spectroscopies I **(FH)**	T
	11h30 – 12h15	Many-Body: GW I **(MV)**	T
	15h00 – 17h30	Introduction to the practical classes	T/P
	18h00 – 21h00	Quantum Dots I	P
2 (4/1)	8h30 – 9h15	TDDFT III **(EG)**	T
	9h30 – 10h15	Overview of spectroscopies II **(FH)**	T
	10h30 – 11h15	Theoretical spectroscopy **(SB)**	T
	11h30 – 12h15	TDDFT IV **(EG)**	T
	15h00 – 17h30	Discussion groups	T/P
	18h00 – 21h00	Quantum Dots II	P
3 (5/1)	8h30 – 16h30	Discussion groups	T/P
	16h30 – 17h15	Many-Body: GW II **(MV)**	T
	17h30 – 18h15	Linear response theory **(SB)**	T
	18h30 – 19h15	Overview of spectroscopies III **(FH)**	T
	19h30 – 20h15	Propagation schemes **(AC)**	T
4 (6/1)	8h30 – 9h15	TDDFT in chemistry and biochemistry I **(BC)**	T
	9h30 – 10h15	Spectroscopy of surfaces **(EO)**	T
	10h30 – 11h15	Overview of spectroscopies IV **(FH)**	T
	11h30 – 12h15	Models for time-dependent phenomena I **(ML)**	T
	15h00 – 18h00	Quantum Dots III	P
	18h30 – 20h30	Poster session	T
5 (7/1)	8h30 – 9h15	Models for time-dependent phenomena II **(ML)**	T
	9h30 – 10h15	TDDFT in chemistry and biochemistry II **(BC)**	T
	10h30 – 11h15	TD Current DFT I **(CU)**	T
	11h30 – 12h15	Many-Body: BSE I **(MG)**	T
	15h00 – 18h00	OCTOPUS I	P
	18h30 – 20h30	Poster session	T
6 (8/1)	8h30 – 15h00	Discussion groups	T/P
	15h00 – 15h45	Advanced TDDFT I **(NM)**	T
	15h45 – 16h30	Optimal control theory **(AC)**	T
	16h45 – 17h30	Models for time-dependent phenomena III **(ML)**	T
	17h30 – 18h15	TD Current DFT II **(CU)**	T
	18h15 – 21h15	OCTOPUS II	P
7 (9/1)	8h30 – 9h15	Models for time-dependent phenomena IV **(ML)**	T
	9h30 – 10h15	Advanced TDDFT II **(NM)**	T
	10h30 – 11h15	Many-Body: BSE II **(MG)**	T
	11h30 – 12h15	TDDFT in chemistry and biochemistry III **(DR)**	T
	15h30 – 20h30	YAMBO	P
8 (10/1)	8h30 – 16h30	Discussion groups	T/P
	16h30 – 17h15	TDDFT versus Many-Body **(MG/AR)**	T
	17h30 – 18h15	TDDFT in chemistry and biochemistry IV **(DR)**	T
	18h30 – 19h15	TD Current DFT III **(CU)**	T
	19h30 – 20h15	Advanced TDDFT III **(NM)**	T
	20h15 – 20h45	Closing session / Pedro Pascual Prize 2010 (organisers: **AR**, **MM**, **FN**, **EG**)	

School Lecturers

Lecturers for the theoretical classes

AC A. Castro (Zaragoza, Spain)
Propagation schemes + Optimal control theory

AR A. Rubio (Donostia/San Sebastian, Spain)
TDDFT vs. Many-Body

BC B. Curchod (Lausanne, Switzerland)
TDDFT in chemistry and biochemistry

CU C. Ullrich (Missouri, USA)
TD Current DFT

DR D. Rappoport (Harvard, USA)
TDDFT in chemistry and biochemistry

EG E. K. U. Gross (MPI Halle, Germany)
TDDFT

EO E. Ortega (Donostia/San Sebastian, Spain)
Spectroscopy of surfaces

FH F. Himpsel (Madison, USA)
Overview of spectroscopies

MG M. Gatti (Paris, France)
Many-Body: BSE + TDDFT vs. Many-Body

ML M. Lein (MPI Heidelberg, Germany)
Models for time-dependent phenomena

MV M. Verstraete (Liège, Belgium)
Many-Body: GW

NM N. Maitra (New York, USA)
Advanced TDDFT

SB S. Botti (Paris, France)
Linear Response Theory + Theoretical spectroscopy

Teachers for `Quantum Dots` and `octopus`

AC Alberto Castro (Zaragoza, Spain)

AR Angel Rubio (San Sebastian, Spain)

FN Fernando Nogueira (Coimbra, Portugal)

MM Miguel Marques (Lyon, France)

MO Micael Oliveira (Lyon, France)

XA Xavier Andrade (San Sebastian, Spain)

Teachers for `YAMBO`

AM Andrea Marini (Rome, Italy)

CO Conor Hogan (Rome, Italy)

DV Daniele Varsano (Modena, Italy)

PG Claudio Attaccalite (San Sebastian, Spain)

MG Myrta Grüning (Coimbra, Portugal)

Workshop Program

Day I: Monday 11th		
Chairperson: Angel Rubio		
09h20 - 09h30	A. Rubio	Opening remarks
09h30 - 10h20	S. Kuemmel	Excitations in finite systems: pragmatic improvements of DFT and fundamental
10h20 - 11h10	C. Cardoso	Long-range correction effects on the evaluation of first hyperpolarizability of high intrinsic hyperpolarizability molecules
11h10 - 11h30	Caffeine break	
Chairperson: Angel Rubio		
11h30 - 12h20	C. Ullrich	Time-dependent density-functional theory for weakly disordered systems: application to dilute magnetic semiconductors
12h20 - 13h10	O. Gritsenko	Time-dependent density matrix functional theory: an interacting alternative to TDDFT
13h10 - 17h20	Discussion groups	
Chairperson: Fernando Nogueira		
17h20 - 18h10	M. Gatti	Sodium under pressure: a charge-transfer insulator
18h10 - 19h00	S. Botti	Electronic properties of materials for thin-film solar cells: Which ab-initio approaches can we trust?
19h00 - 19h20	Beer break	
Chairperson: Fernando Nogueira		
19h20 - 20h10	J. Dobson	Applications of RPA, TDDFT and related response functions to correlation energies
20h10 - 21h00	E. Suraud	TDDFT description of irradiation and the Self Interaction Problem
Day II: Tuesday 12th		
08h30 - 17h00		Mini-workshops
Chairperson: Mark Casida		
17h00 - 17h50	T. Seideman	Why Time-Dependent Density Functional Theory?
17h50 - 18h40	N. Maitra	Phase-Space Density Dynamics
18h40 - 19h00	Beer break	
Chairperson: Mark Casida		
19h00 - 19h50	R. Baer	Pragmatic and Dogmatic Spirits in Time-Dependent Density Functional Theory
19h50 - 20h40	I. Tokatly	Time-dependent deformation functional theory: From basic theorems to first applications

Day III: Wednesday 13th		
Chairperson: Miguel Marques		
08h30 - 09h20	M. Sprik	Electronic energy levels in liquids and near liquid-solid interfaces: An electrochemical perspective
09h20 - 10h10	I. Tavernelli	Non-adiabatic molecular dynamics with external fields
10h10 - 10h30	Caffeine break	
Chairperson: Miguel Marques		
10h30 - 11h20	H. Appel	Stochastic Quantum Molecular Dynamics: a functional theory for electrons and nuclei dynamically coupled to an environment
11h20 - 12h10	R. D'Agosta	Stochastic time dependent (current) density functional theory: fundaments and applications
12h10 - 13h00	O. Sugino	Non-adiabatic molecular simulations
13h00 - 17h00	Discussion groups	
17h00 - 18h30	Poster session	
Chairperson: John Dobson		
18h30 - 19h20	M. Casida	The Multifaceted Problem of Double- and Higher-Excitations in TDDFT
19h20 - 20h10	A. Goerling	New Developments in Density-Functional Response Methods and new Correlation Functionals
20h10 - 21h00	T. Niehaus	Inverse quantum confinement in luminescent Silicon quantum dots

Day IV: Thursday 14th		
Chairperson: Carsten Ullrich		
16h00 - 16h50	F. Martin	Kinematically complete theoretical description of molecular ionization by synchrotron radiation and ultrashort pulses
16h50 - 17h40	C. Ambrosch-Draxl	Q-dependent TDDFT spectra from metals
17h40 - 18h10	D. Strubbe	Non-linear optics and local-field factors in liquid chloroform: A time-dependent density-functional theory study *Winner of the school poster session*
18h10 - 18h30	Beer break	
Chairperson: Stephan Kuemmel		
18h30 - 19h00	G. Avendaño-Franco	Time-Dependent Density Functional Theory study of transfer of charge by atomic impact, a case study with C4H20 + Au *Winner of the school poster session*
19h00 - 19h50	P. Umari	GW quasi-particle spectra from occupied states only
19h50 - 20h00	A. Rubio	Closing remarks
21h00 -		Workshop dinner

List of Students

Péter ÁGOSTON	Technical University Darmstadt
Joseba ALBERDI	EHU/UPV and ETSF
Guillermo AVENDAÑO FRANCO	Université Catholique de Louvain
Fulvio BERARDI	EHU/UPV and ETSF
Robertson BURGESS	The University of Newcastle
Pablo CAMPOMANES RAMOS	Ecole Polytechnique Federale Lausanne (EPFL)
Elena CANNUCCIA	Universitá di Roma Tor Vergata
Vince CHO	Norhtwestern University
Pierluigi CUDAZZO	UPV/EHU
Ingo DREIßIGACKER	Leibniz Universität Hannover
Luiza EPURE	Technical University "Gh.Asachi"
Corina ETZ	MPI for Microstructure Physics Halle
James FINN	King's College London
Johanna FUKS	Universidad del Pais Vasco
Pablo GARCIA	Universidad de Zaragoza
Tahereh GHANE	Natl. Center S3 INFM-CNR
Prasenjit GHOSH	The Abdus Salam ICTP
Marco GOVONI	University of Modena and Reggio Emilia
Prokop HAPALA	Inst. of Phys. of the Academy of Sc. of Czech Republic
S. M. Javad HASHEMI	Helsinki University of Technology
Miquel HUIX-ROTLLANT	Université Joseph Fourier (Grenoble I)
Amilcare IACOMINO	Università degli Studi Roma Tre
Federico IORI	Ecole Polytechnique
Olexandr ISAYEV	Case Western Reserve University
Dominik JOCHYM	STFC Rutherford Appleton Laboratory
Deniz KECIK	Paul Scherrer Institute
MANOJ KUMAR	University of Louisville
Aritz LEONARDO LICERANZU	University of Missouri
Pablo LOPEZ TARIFA	Universidad Autónoma de Madrid
Sergio Alberto LOSILLA FERNÁNDEZ	University of Helsinki
Ruskan MINIBAEV	Photochemistry Center of Russian Academy of Science
S. Hossein MIRHOSSEINI	Max-Planck-Institut für Mikrostrukturphysik
Asmaâ MOUJIB	Mohammed V University Agdal
Bhaarathi NATARAJAN	Université Joseph Fourier (Grenoble I)
Danilo NITSCHE	Freie Universität Berlin
David OREGAN	Cavendish Laboratory / University of Cambridge
Rengin PEKÖZ	Universite de Liege
Anna PERTSOVA	Trinity College Dublin
James RAMSDEN	The University of York
Laurids SCHIMKA	University of Vienna
Estelina Lora SILVA	University of Aveiro
John SNYDER	University of California
David STRUBBE	University of California
David TEMPEL	Harvard University
Gilberto TEOBALDI	University College London
Omar VALSSON	University of Twente
Alejandra VARGAS CALDERÓN	CINVESTAV Querétaro
Feng WANG	Institute of Modern Physics

List of School Teachers

Xavier Iago ANDRADE VALENCIA	Universidad del Pais Vasco
Claudio ATTACCALITE	Universidad del Pais Vasco
Silvana BOTTI	LSI-Laboratoire des Solides Irradiés
Alberto CASTRO	Free University of Berlin / BIFI
Hogan CONOR	Universitá di Roma Tor Vergata
Basile CURCHOD	École Polytechnique Fédérale
Matteo GATTI	ETSF and UPV - Universidad del Pais Basco
E. K. U. GROSS	FU Berlin
Myrta GRÜNING	Universidade de Coimbra
Franz HIMPSEL	University of Wisconsin Madison
Manfred LEIN	Universität Hannover
Neepa MAITRA	Hunter College of the City University of New York
Andrea MARINI	Universitá di Roma Tor Vergata
Miguel MARQUES	LPMCN - Université Lyon I
Fernando NOGUEIRA	Universidade de Coimbra
Micael OLIVEIRA	LPMCN - Université Lyon I
Enrique ORTEGA	UPV - Universidad del Pais Basco
Dmitrij RAPPOPORT	Harvard University
Angel RUBIO	UPV – Universidad del Pais Vasco
Carsten ULLRICH	University of Missouri
Daniele VARSANO	National Center CNR-INFM S3
Matthieu VERSTRAETE	Universidad del Pais Vasco

List of Workshop Participants
(besides the students and teachers from the school)

Akbari ALI	Universidad del País Vasco
Claudia AMBROSCH-DRAXL	University of Leoben
Heiko APPEL	University of California
Roi BAER	The Hebrew University of Jerusalem
Leonardo BERNASCONI	STFC Rutherford Appleton Laboratory
Cláudia CARDOSO	Universidade de Coimbra
Mark CASIDA	Université Joseph Fourier (Grenoble I)
Roberto D'AGOSTA	EHU/UPV and ETSF
John DOBSON	Griffith University
Juan Maria GARCIA-LASTRE	EHU/UPV and ETSF
Andreas GOERLING	University of Erlangen-Nuremberg
Oleg GRITSENKO	Free University Amsterdam
Nicole HELBIG	EHU/UPV and ETSF
Hirotoshi HIRAI	University of Tokyo
Stephan KUMMEL	University of Bayreuth
Stefan KURTH	Free University of Berlin
Espinosa LEONARDO	University of the Basque Country and ETSF
Fernando MARTIN	Universidad Autonoma de Madrid
Thomas NIEHAUS	Universität Bremen
Yann POUILLON	Universidad del Pais Vasco
Tamar SEIDEMAN	Northwestern University
Michiel SPRIK	University of Cambridge
Tamar STEIN	The Hebrew University of Jerusalem
Osamu SUGINO	ISSP
Eric SURAUD	Université Paul Sabatier
Ivano TAVERNELLI	Ecole Poly. Fédérale de Lausanne (EPFL)
Ilya TOKATLY	Universidad del Pais Vasco UPV/EHU and ETSF
Paolo UMARI	INFM crs Democritos
Jessica WALKENHORST	Universität Kassel
Marius WANKO	University of Bremen
Zeila ZANOLLI	Universite' catholique de Louvain

TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY: PROSPECTS AND APPLICATIONS

4th International Workshop and School

Benasque (Spain), January 2 – 15, 2010

A. Rubio (Univ. País Vasco and ETSF, Spain),
E. K. U. Gross (MPI Halle, Germany),
M. A. L. Marques (LPMCN, Université Lyon I, France),
F. Nogueira (CFC and Univ. de Coimbra, Portugal)

Supported by:

Workshop Invited Talks

Excitations in finite systems: pragmatic improvements of DFT and fundamental questions in TDDFT

Stephan Kümmel

Theoretische Physik
Universität Bayreuth
D-95440 Bayreuth
Germany

Molecular organic semiconductors are examples of many electron systems for which the accurate prediction of excitations is of great practical interest, e.g., for understanding organic solar cells. A parameter-free and well working self-interaction correction approach to calculate photoelectron spectra for these systems will be discussed. This pragmatic approach will be contrasted with efforts to improve rigorous TDDFT by obtaining insights from simple model systems. We constructed the adiabatically exact exchange-correlation kernel numerically and demonstrate the consequences that even the "best possible adiabatic approximation" has on the excitation spectrum.

Long-range correction effects on the evaluation of first hyperpolarizability of high intrinsic hyperpolarizability molecules

Cláudia Cardoso

Centro de Física Computacional, Universidade de Coimbra
Portugal

Time-dependent density-functional theory for weakly disordered systems: application to dilute magnetic semiconductors

Carsten A. Ullrich

University of Missouri
USA

We present a theory for transport and optical response in disordered systems, based on an equation-of-motion approach for the current-current response function [1-3]. The resulting formalism combines a TDDFT treatment of the current response in a clean reference system with a self-consistent description of disorder scattering caused by charged and magnetic impurities beyond the relaxation-time approximation. In practice we evaluate the formalism in the weak disorder limit, using a multiband k.p description of the host semiconductor material.

In III-V dilute magnetic semiconductors (DMS) such as GaMnAs, the transition-metal impurities are responsible both for providing mobile hole carriers and for inducing ferromagnetic transitions. This leads to rich and complex scenarios for optical and transport properties, where impurity scattering and many-body effects play an equally important role. We discuss the effects of exchange-correlation, dynamic screening and collective electron excitations on the charge and spin scattering off Coulomb impurities and fluctuations of localized spins. We show that the exchange-correlation effects play an important role in the temperature dependence of dc-conductivity in DMS. Collective, plasmon-like excitations within the hole liquid substantially modify the carrier scattering rate at finite frequencies. The so calculated infrared optical conductivities of GaMnAs compare well with experimental data [4].

This work was supported by DOE grant DE-FG02-05ER46213.

[1] F. V. Kyrychenko and C. A. Ullrich, Phys. Rev. B 80, 205202 (2009)

[2] F. V. Kyrychenko and C. A. Ullrich, J. Phys.: Condens. Matter 21, 084202 (2009)

[3] F. V. Kyrychenko and C. A. Ullrich, Phys. Rev. B 75, 045205 (2007)

[4] E. J. Singley, K. S. Burch, R. Kawakami, J. Stephens, D. D. Awschalom, and D. N. Basov, Phys. Rev. B 68, 165204 (2003)

Time-dependent density matrix functional theory: an interacting alternative to TDDFT

O.V. Gritsenko, K.J.H. Giesbertz, E.J. Baerends

Vrije Universiteit Amsterdam
and POSTECH, Pohang, Korea

Excitons in dense sodium

Matteo Gatti, Ilya Tokatly, and Angel Rubio

EHU/UPV — Universidad del Pais Vasco, Donostia/San Sebastian
Spain
and European Theoretical Spectroscopy Facility

At ambient conditions sodium is the prototype of a nearly free-electron metal. Under pressure one would expect an increase of the bandwidth and hence a more free-electron-like behavior. Instead, at high pressure, sodium undergoes a phase transition becoming an insulator with a large gap [1,2].

Here we study excitonic effects in the absorption spectrum of the insulating phase of sodium. We discover an unusual kind of charge-transfer exciton that proceeds from the interstitial distribution of valence electrons repelled away from the ionic cores by the Coulomb interaction and the Pauli repulsion. The predicted absorption spectrum shows a strong anisotropy with light polar- ization that just at pressures above the metal-insulator transition manifests as sodium being optically transparent in one direction but reflective in the other. This result provides a key information for an experimental conclusive deter- mination of the crystal structure of transparent sodium, a new unconventional inorganic electride.

[1] B. Neaton and N. W. Ashcroft, PRL **86**, 2830 (2001).

[2] Y. Ma *et al.*, Nature **458**, 182 (2009).

Electronic properties of materials for thin-film solar cells: Which ab initio approaches can we trust?

Silvana Botti

LSI — Ecole Polytechnique, Palaiseau
France

During the past years, $Cu(In,Ga)(Se,S)_2$ (CIGS) thin-film solar cells emerged as a technology that could challenge the current hegemony of silicon solar panels. CIGS compounds conserve to a very high degree their electronic properties in a large non-stoichiometric range and are remarkably insensitive to radiation damage or impurities. Moreover, thin film solar cells require transparent contacts. In practice, these contacts are built from insulating oxides that for a certain range of doping become conductive while retaining transparency in the visible spectrum. Thin films of compounds of the delafossite family, namely $Cu(Al,Ga,In)O_2$, are particularly interesting as they show bipolar conductivity.

The origin of the exceptional electronic properties of these two classes of materials is still not well understood, despite the large amount of experimental and theoretical works dedicated to this purpose. This is a serious restraint when it comes to designing new materials for more efficient photovoltaic energy conversion.

In this context, can ab-initio calculations of electronic excitations give a crucial contribution? Which theoretical approaches are reliable?

In my talk I will try to give an answer to these questions.

Applications of RPA, TDDFT and related response functions to correlation energies

Sebastian Lebegue, Tim Gould, Julien Toulouse, Janos Angyan, John Dobson, Judith Harl, Georg Kresse, Angel Rubio

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We discuss some recent applications of RPA response, and beyond, in applications such as electronic groundstate energy and van der Waals C6 coefficients. Results to be discussed include the net layer binding energy and stretching curve of graphite, and some data about dynamic and groundstate screening in time dependent linear response of atoms.

TDDFT description of irradiation and the Self Interaction Problem

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Why Time-Dependent Density Functional Theory?

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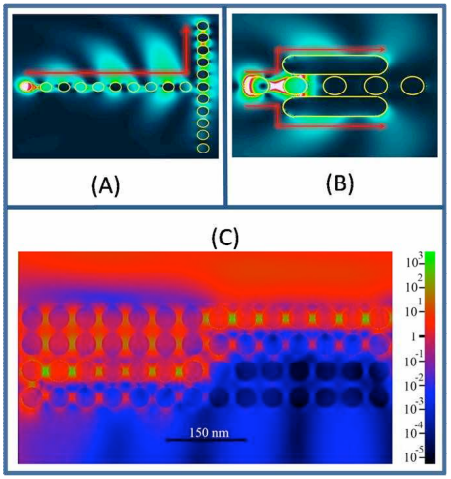
We discuss directions and opportunities for TDDFT in future research. Specifically, we highlight several fields of contemporary research where we expect TDDFT to have a role in future theories. One such instance, with which the audience of the present workshop is familiar, is transport calculations via molecular nanojunctions, where interesting nonequilibrium effects call for theories that go beyond static DFT. Closely related is the emerging field of current-driven dynamics in molecular-scale electronics, where strongly nonadiabatic physics combine with resonance scattering to suggest the potential of quantum theories that go beyond the Born-Oppenheimer approximation. A third topic of growing interest is the problem of nanoplasmonics—the interaction of light with metal nanoparticles and their arrays, where quantum effects play an increasingly significant role as the particle size decreases, calling for theories that go beyond classical electrodynamics. We conclude with a discussion of

electron dynamics in strong laser fields, a fascinating problem in theoretical research which manifests itself in phenomena ranging from high harmonic generation to double ionization, and where current theories struggle to account for the 3D large amplitude electronic dynamics and the consequences of correlation.



Several of the applications we envision in the field of nanoplasmonics, for instance, are schematically illustrated in the figure. The T-junction of Fig. 1A guides electromagnetic energy traveling down the leg into one or the other of the two symmetry- equivalent arms of the junction. Figure 1B depicts a hybrid construct, which combines elements that provide local enhancement with elements that provide long distance propagation in order to minimize losses. The structural parameters of the construct are optimized using a genetic algorithm. Fig. 1C depicts a plasmonic nanocrystal, developed to separate an incident plane wave into two frequency components and funnel each component in a different direction normal to the direction of incidence.

Phase-Space Density Dynamics

Neepa Maitra

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Pragmatic and Dogmatic Spirits in Time-Dependent Density Functional Theory

Roi Baer

Dept. of Physical Chemistry, The Hebrew University
Israel

Time-dependent deformation functional theory: From basic theorems to first applications

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EHU/UPV — Universidad del Pais Vasco, Donostia/San Sebastian
Spain

In this talk I discuss the time-dependent deformation functional theory (TDDefFT) – a recently proposed approach to the many-body dynamics, which uses a deformation tensor of the electron liquid as a basic variable. In general TDDefFT can be viewed as a version (or a refinement) of the time-dependent current density functional theory. However, in contrast to the standard DFT-like theories, the exact formulation of TDDefFT avoids a traditional potential-to-density mapping. Instead the theory can be formulated in a form similar to the ground-state constrained search procedure. Within this formalism all basic functionals appear from the solution of a constrained universal many-body problem in a co-moving reference frame, which is equivalent to finding a conditional extremum of a certain universal action functional.

I also review some recent application of TDDefFT, such as, a closed quantum continuum mechanics for many-body systems – a non-Kohn-Sham approach the the linear dynamics; the derivation of the exact anti-adiabatic limit for the xc kernel in TDDFT, and ab-initio calculations of the coefficient in the phenomenological $1/q^2$ kernel proposed to describe excitonic effects in semiconductors.

Aligning electronic energy levels in liquids, solids and their interfaces: An electrochemical perspective

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In practical applications time dependent density functional theory is often used as a perturbative correction applied to one-electron (Kohn-Sham) orbitals obtained form time independent density functional theory (DFT in short). While optical excitation energies formally depend on differences between energies of virtual and occupied orbitals, the question of the absolute position of the levels is still relevant. For example, if the orbital energy gaps are a bad approximation to the optical excitation energies, which is often the case when the virtual states are delocalized, it could be helpful to know whether this is due to the empty or occupied orbitals or both. The for chemical applications most relevant orbitals are the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The experimental observables correlated with HOMO and LUMO energies are the minimum ionization potential (IP) respectively the maximum electron afnity (EA).

The question of absolute positions of energy levels is crucial when comparing the density of states of two different condensed phases. This so-called level alignment problem is particularly hard when it concerns delocalized band states of solids and localized molecular states in liquids. This is where the GGA level DFT approximations used in extended system calculations are least reliable. Furthermore for liquids we cannot ignore the distinction between the adiabatic and vertical IP's and EA's. An adiabatic IP (by definition equal to the corresponding adiabatic EA) can be estimated by converting

the reduction potentials measured by electrochemical methods to an absolute (vacuum) scale. The HOMO of a solvated molecule, however, must be compared to the vertical IP as measured by PES methods. The differences between vertical and adiabatic IP's can be very large (up to 3eV in aqueous systems[1]) due to the reorganization of the solvent.

We have approached this problem using DFT based molecular dynamics simulation (DFTMD) of fully atomistic model systems under periodic boundary conditions. IP's and EA's are computed as the relative total energy of two systems with one electron less (or more). For solids the energies are referred to vacuum using a solid-vacuum interface as model system conform the practice in computational surface chemistry, The energies in liquids, however, are directly determined relative to the normal hydrogen electrode [1] in a homogeneous model system using an extension of the reversible proton insertion method we have developed for the computation of acidity constants[2,3]. The same method can also be applied to solid (electrode)-liquid (electrolyte) interfaces in a repeated liquid- solid slab geometry. These techniques will be illustrated in this talk by an application to the interface between an alkaline electrolyte and titania (TiO2). One of the results of these (still ongoing) calculations is that for the PBE functional the bottom of the conduction band of titania is in fair agreement with the experimental flatband potential once the 1 eV upward shift in the titania energy levels as a result of hydration is taken into account. Since the PBE band gap is too small by at least an eV, this unfortunately means that the top of the valence band ends up too high, in fact above the adiabatic IP we calculated for OH-/OH° in homogeneous solution[1], in painful disagreement with experiment.

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Non-adiabatic molecular dynamics with external fields

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Stochastic Quantum Molecular Dynamics: a functional theory for electrons and nuclei dynamically coupled to an environment

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Stochastic time dependent (current) density functional theory: fundaments and applications

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Ikerbasque and EHU/UPV — Universidad del Pais Vasco, Donostia/San Sebastian
Spain

Static and dynamical density functional methods have been applied with a certain degree of success to a variety of closed quantum mechanical systems, i.e., systems that can be described via a Hamiltonian dynamics. However, the relevance of open quantum systems - those coupled to external environments, e.g., baths or reservoirs - cannot be overestimated. To investigate open quantum systems with DFT methods we have introduced a novel theory, we have named Stochastic Time-Dependent Current Density Functional theory (S-TDCDFT). In this talk, I will introduce the stochastic formalism needed for the description of open quantum systems, discuss in details the theorem of Stochastic TD-CDFT, the connection of the theory with a density matrix formalism, and provide few examples of its applicability like the dissipative dynamics of excited systems, quantum-measurement theory and other applications relevant to charge and energy transport in nanoscale systems.

Non-adiabatic molecular simulations

Osamu Sugino

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The Multifaceted Problem of Double- and Higher-Excitations in TDDFT

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The conventional approach to extracting information about electronic excited states from time- dependent density-functional theory (TDDFT) [1] makes use of the TDDFT adiabatic approximation (AA) which assumes that the self-consistent eld responds instantaneously and without memory to any temporal change in the charge density. Electronic excitation spectra may then be obtained by linear response (LR) theory using, for example, Casida's equation [2] in the energy representation. It is now

well-established that the AA restricts LR-TDDFT to single-electron quasiparticle excitations. However explicit two- and higher-electron excitations are needed to describe a number of highly interesting excited-state problems, some of which will presented in more or less detail as time allows:

- AA LR-TDDFT leads to spin-contamination in some excited states of open-shell molecules, such as [Fe(H2 O)6]2+ [3, 4].

- Polarization propagator theory provides insight into the analytic structure of the exact exchange-correlation (xc) kernel, fxc(ω) [5]. This provides an improved understanding of dressed TDDFT [6].

- Biradicaloid ground states enter into photochemical problems involving avoided crossings and conical intersections. Ground singlet-state referenced TDDFT requires us to overcome an effective noninteracting v-representability problem. Excited triplet-state referenced spin-ip TDDFT encounters other problems [7].

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New Developments in Density-Functional Response Methods and new Correlation Functionals

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Inverse quantum confinement in luminescent Silicon quantum dots

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Kinematically complete theoretical description of molecular ionization by synchrotron radiation and ultrashort pulses

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The performance of TDDFT for excitation spectra of solids: From optical propierties and electron energy loss of simple metals to core - excitations in large gap materials

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Non-linear optics and local-field factors in liquid chloroform: A time-dependent density-functional theory study

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ETSF and Centro de Física de Materiales, Universidad del Pais Vasco, San Sebastian, Spain

Time-Dependent Density Functional Theory study of transfer of charge by atomic impact, a case study with C_4H_{20} + Au

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GW quasi-particle spectra from occupied states only

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School Poster Session

Using Hydrogenic Orbitals to Improve DFT

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In Density Functional Theory (DFT), the Hohenberg-Kohn theorem allows us to map the interacting system to a fictitious non-interacting Kohn-Sham system, with an effective one-body potential, that reproduces the groundstate density of the interacting system. Formally, this mapping is exact, which suggests that studying the non-interacting system may provide useful insight into the interacting system. We use the Bohr atom, with non-interacting electrons in hydrogenic orbitals, as a model to find the asymptotic expansion of its exchange energy in a charge-neutral scaling as atomic number Z approaches infinity. We show that, like in the interacting atom, B88 and PBE are close to having the correct asymptotic form, while GE2 is off by a factor of 2. We adjust the parameter in GE2 to enforce the correct asymptotic form. We have also developed a new piecewise smooth model for the density of the Bohr atom that improves upon the Thomas-Fermi density.

Non-linear optics and local-field factors in liquid chloroform: A time-dependent density-functional theory study

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Time-Dependent Density Functional Theory study of transfer of charge by atomic impact, a case study with C_4H_{20} + Au

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Optical Property Calculations of Gold-based Alloys with Density Functional Theory

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Excitations from Open Quantum Systems TDDFT

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Structure and Dynamics of Bacterial Nitroreductase

Olexandr Isayev, Leonid Gorb, Narimantas Cenas, Frances Hill and Jerzy Leszczynski

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Jackson State University, Jackson, USA and
Institute of Biochemistry, Vilnius, Lithuania

A strong correlation study: the paradigmatic case of the V_2O_3

Federico Iori, Matteo Gatti, and Lucia Reining

Ecole Polytechnique, Palaiseau, France and ETSF

Azopolysiloxanes modified with nucleobases, systems with potential applications in DNA immobilization and nanomanipulation processes

Elena-Luiza Epure and Nicolae Hurduc

Technical University of Iasi, Romania

Water clusters in atmosphere

J. Finn

King's College London, UK

Explicit Double-Excitations in TDDFT

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Photoisomerization of model retinal chromophores: Insight from quantum Monte Carlo and multiconfigurational perturbation theory

Omar Valsson and Claudia Filippi

Faculty of Science and Technology and MESA+ Research Institute
University of Twente, The Netherlands

Optical properties of DNA-derivatives for nanoelectronics applications

Tahereh Ghane, Daniele Varsano, Giorgia Brancolini, Elisa Molinari and Rosa Di Felice

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CO Adsorption on Transition Metal Surfaces Applying the Random Phase Approximation

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TDDFT Calculations of the Optical Properties of Metallic Particles

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Accurate electrostatic potentials for periodic systems

Sergio A. Losilla, Dage Sundholm, and Jonas Jusélius

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University of Tromso, Norway

Ab-initio calculation of the Impact Ionization Rate in GaAs using yambo code

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Electronic Properties of Doped Silicon Nanocrystals

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Role of Tyrosine Residue in the activation of Co-C bond in Coenzyme B_{12}-Dependent Enzimes: Another case of Proton-Coupled Electron Transfer?

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Defective carbon nanotubes: magnetism, spin transport and gas sensing applications

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Carbon nanotubes (CNTs) are renowed in the scientic community for being both a playground for studying fundamental physical properties and for applications in, to mention a few, electronic, spintronic and gas sensing technologies. However, despite the progresses in growth techniques, CNTs always exhibit structural defects [1] and their electronic and transport properties will be aected accordingly [2]. In addition, the presence of defects in carbon-based nanostructures has been seen as source of magnetism [3]. Hence, mastering the physics underlying defected CNTs is crucial not only to model realistic systems but also to design new devices.

The spin-polarized electron transport properties of carbon nanotubes with vacancies are investigated using rst principles and non-equilibrium Green's function techniques [4]. Carbon atoms with unsaturated bonds are found to behave as quasi-localized magnetic impurities, coupled by long range interactions. The magnetism of carbon nanotubes with reconstructed mono- and tri-vacancies results in spin dependent contuctances and, hence, can be exploited in spintronic devices such as nano-spin valves.

Clarified the properties of CNTs with vacancies, the sensing ability of defected CNTs towards several molecules (NO2 , NH3 , CO, CO2 , H2 O) has also been investigated ab initio. Since the adsorption/desorption of molecules induces modulations on the electrical conductivity of the tube, quantum conductances of the CNT-based sensors are predicted, nding that defective nanotubes are sensitive to NO2 , NH3 and CO, while molecular selectivity is provided by the nature of the charge transfer.

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Time-Dependent Density-Functional Theory with Finite Elements

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Optical gap of semiconductors and oxides from Coupled Perturbed Hartree-Fock and Coupled Perturbed Kohn-Sham theory

Leonardo Bernasconi, Stanko Tomic and Nicholas M. Harrison

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Time-Dependent Range-Separated Hybrid Functionals for the description of Molecular Charge Transfer States

Tamar Gershon, Leeor Kronik, and Roi Baer

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Modeling radiation-damage processes in organic solids via DFT calculations of EMR parameters

H. De Cooman, E. Pauwels, H. Vrielinck, E. Sagstuen, F. Callens, and M. Waroquier

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MR. DAVID A. STRUBBE HAS BEEN AWARDED 1ST PRIZE IN THE SECOND PEDRO PASCUAL CONTEST FOR THE BEST POSTER PRESENTED DURING THE FOURTH SUMMER SCHOOL "TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY: PROSPECTS AND APPLICATIONS" HELD IN BENASQUE FROM THE 2ND TO THE 15TH OF JANUARY 2010.

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