3.1.2 Report on 3rd International Workshop and School on Time-Dependent Density Functional Theory: Prospects and Applications

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

Organized by
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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 PAscula Prize for the best posters of the school). 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 participated 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
Male PhD	27	2		2	31
Female PhD	9				9
PhD	**36**	**2**		**2**	**40**
Male Post-doc	11	21	13	7	52
Female Post-doc	3	2	3	4	12
Post-doc	**14**	**23**	**16**	**11**	**64**
Male	38	23	13	9	83
Female	12	2	3	4	21
# Participants	**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, appli-

cations 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) Material Science, Nanosciecen, 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 (1/9)	9h30 – 10h15	TDDFT I **(EG)**	T
	10h30 – 11h15	TDDFT II **(EG)**	T
	11h30 – 12h15	Overview of spectroscopies I **(MC)**	T
	12h30 – 13h15	Many-Body: GW I **(RG)**	T
	15h00 – 18h30	Introduction to the practical classes	P
2 (2/9)	9h30 – 10h15	Overview of spectroscopies II **(MC)**	T
	10h30 – 11h15	TDDFT III **(EG)**	T
	11h30 – 12h15	Many-Body: GW II **(RG)**	T
	12h30 – 13h15	Theoretical spectroscopy **(SB)**	T
	15h00 – 18h30	Quantum Dots I	P
3 (3/9)	9h30 – 10h15	TDDFT IV **(EG)**	T
	10h30 – 11h15	Overview of spectroscopies III **(MC)**	T
	11h30 – 12h15	Propagation schemes **(AC)**	T
	12h30 – 13h15	Linear response theory **(SB)**	T
	15h00 – 18h30	Quantum Dots II	P

4 (4/9)	9h30 – 10h15	Advanced TDDFT I **(NM)**	T
	10h30 – 11h15	Current DFT I **(CU)**	T
	11h30 – 12h15	Overview of spectroscopies IV **(MC)**	T
	12h30 – 13h15	TDDFT as a tool in chemistry I **(IT)**	T
	15h00 – 18h30	Quantum Dots III	P
5 (5/9)		Free day	
6 (6/9)	9h30 – 10h15	TDDFT as a tool in chemistry II **(IT)**	T
	10h30 – 11h15	Current DFT II **(CU)**	T
	11h30 – 12h15	Many-Body: BSE I **(MG)**	T
	12h30 – 13h15	Advanced TDDFT II **(NM)**	T
	15h00 – 18h30	OCTOPUS I	P
	18h30 – 19h30	Max Planck - A conservative revolutionary **(MC)**	Public talk
7 (7/9)	9h30 – 10h15	TDDFT as a tool in chemistry III **(IT)**	T
	10h30 – 11h15	Many-Body: BSE II **(MG)**	T
	11h30 – 12h15	Current DFT III **(CU)**	T
	12h30 – 13h15	Optimal control theory **(AC)**	T
	15h00 – 18h30	OCTOPUS II	P
	18h30 – 20h00	Posters	
8 (8/9)	9h30 – 10h15	TDDFT versus Many-Body I **(RvL)**	T
	10h30 – 11h15	TDDFT as a tool in biophysics I **(ME)**	T
	11h30 – 12h15	Advanced TDDFT III **(NM)**	T
	12h30 – 13h15	TDDFT as a tool in biophysics II **(ME)**	T
	15h00 – 18h30	YAMBO I	P
	18h30 – 20h00	Posters	
9 (9/9)	9h30 – 10h15	Nonlinear optics **(XA)**	T
	10h30 – 11h15	TDDFT versus Many-Body II **(RvL)**	T
	11h30 – 12h15	TDDFT as a tool in biophysics III **(RS)**	T
	12h30 – 13h15	Fraud in science I **(SO)**	T
	15h00 – 18h30	YAMBO II	P
	18h30 – 19h00	Fraud in science II **(SO)**	T
	19h00 – 19h30	Closing session (organisers: **AR**, **MM**, **FN**, **EG**)	

School Lecturers

Lecturers for the theoretical classes

AC A. Castro (FU Berlin, Germany)
Propagation schemes + Optimal control theory

CU C. Ullrich (Missouri, USA)
Current DFT

EG E. K. U. Gross (FU Berlin, Germany)
TDDFT

IT I. Tavernelli (Lausanne, Switzerland)
TDDFT as a tool in chemistry

MC M. Cardona (Stuttgart, Germany)
Overview of spectroscopies
Public talk: Max Planck - A conservative revolutionary

ME M. Elstner (Braunschweig, Germany)
TDDFT as a tool in biophysics

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

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

RG R. W. Godby (York, UK)
Many-Body: GW

RvL R. van Leeuwen (Groningen, The Netherlands)
TDDFT versus Many-Body

RS R. Send (Irvine, USA)
TDDFT as a tool in biophysics

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

SO S. Ossicini (Modena, Italy)
Fraud in science

XA X. Andrade (San Sebastian, Spain)
Nonlinear optics

Teachers for `Quantum Dots` and `octopus`

AC Alberto Castro (Berlin, Germany)

AR Angel Rubio (San Sebastian, Spain)

FN Fernando Nogueira (Coimbra, Portugal)

MM Miguel Marques (Lyon, France)

MO Micael Oliveira (Coimbra, Portugal and San Sebastian, Spain)

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 Pablo Garcia (Madrid, Spain)

SB Silvana Botti (Paris, France)

YP Yann Pouillon (San Sebastian, Spain)

Workshop Program

Day I: Thursday 11th		
Chairperson: E.K.U. Gross		
09h00 - 09h10	Angel Rubio	Opening remarks
09h10 - 10h00	Kieron Burke	Semiclassical origins of density functional theory
10h00 - 10h50	Roi Baer	Dogmatic and Pragmatic Spirits in TDDFT
10h50 - 11h20	Caffeine break	
Chairperson: Neepa Maitra		
11h20 - 12h10	Marc Casida	TDDFT pushing the limits of and going beyond the adiabatic approximation
12h10 - 13h00	S. Kuemmel	Memory effects in real time: Probing the adiabatic approximation in TDDFT
13h00 - 15h00	Lunch break	
Chairperson: Angel Rubio		
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	M. di Ventra	Stochastic TDCDFT: a functional theory of open quantum systems
13h00 - 15h00	Lunch break	
Chairperson: Kieron Burke		
15h00 - 15h50	R. van Leeuwen	Time-Dependence and Interactions in Quantum Transport
15h50 - 16h40	Risto Nieminen	Applications of TDDFT to clusters and nanostructures
16h40 - 17h10	Beer break	
Chairperson: Ivano Tavernelli		
17h10 - 18h00	Claudia Filippi	Autofluorescent proteins: Are first-principle calculations predictive?
18h00 - 18h50	N. Maitra	TDDFT phase-space explorations
20h00	Speakers Dinner	

Day III: Saturday 13th		
Chairperson: Fernando Nogueira		
09h00 - 09h50	Nikos Doltsinis	Nonadiabatic Car-Parrinello MD
09h50 - 10h40	Osamu Sugino	Nonadiabatic dynamics by TDDFT
10h40 - 11h10	Caffeine break	
Chairperson: Osamu Sugino		
11h10 - 12h00	Ivano Tavernelli	Non-adiabatic mixed quantum-classical dynamics using TDDFT
12h00 - 12h50	Kazuhiro Yabana	Dynamics in dielectrics induced by ultrashort laser pulses
13h00 - 15h00	Lunch break	
Chairperson: Massimiliano di Ventra		
15h00 - 15h50	Troy Van Voorhis	Electron Transfer and Electron Transport: Fighting Self-Interaction in TDDFT
15h50 - 16h40	Daniele Varsano	Optical Saturation driven by Exciton Confinement in Molecular Chains
16h40 - 17h10	Beer break	
Chairperson: Massimiliano di Ventra		
17h10 - 18h00	Silvana Botti	Photoelectronic properties of chalcopyrites for photovoltaic conversion: self-consistent GW calculations
18h00 - 20h00	Poster Session	

Day IV: Sunday 14th		
Chairperson: Miguel Marques		
09h00 - 09h20	Ingolf Warnke	*Winner of the school poster session*
09h20 - 09h40	P. Myhnen	*Winner of the school poster session* Quantum transport studies in Kadanoff-Baym approach
09h40 - 10h30	P. Romaniello	Double excitations in finite systems
10h30 - 11h00	Caffeine break	
Chairperson: Miguel Marques		
11h00 - 11h50	Claudio Verdozzi	TDDFT and Strongly Correlated Systems: Insight From Numerical Studies
11h50 - 12h00	Miguel Marques	Closing remarks

List of Students

Ali AKBARI	Centro Joxe Mari Korta, San Sebastin, Spain
Joice ARAJO	UFMG - Universidade Federal de Minas Gerais
Jakub BARAN	Tyndall National Institute, University College Cork
Christophe BERSIER	FU Berlin (freie universitt)
Oana BUNAU	Institut Neel, CNRS Grenoble, France
Letizia CHIODO	National Nanotechnology Laboratory of CNR-INFM
Stefania D'AGOSTINO	CRS NNL, INFM-CNR, Lecce (ITALY)
Fabiana DA PIEVE	Institut Carnot de Bourgogne, Universit de Bourgogne

Florian EICH	Freie Universitaet Berlin, Berlin, Germany
Leonardo ESPINOSA LEAL	Universidad del Pais Vasco
Jos Rui FAUSTINO DE SOUSA	Universidade de Coimbra
Frederico FIORAVANTI	UFMG - Universidade Federal de Minas Gerais
Dietrich FOERSTER	C.P.M.O.H. Universite de Bordeaux I
Giorgia FUGALLO	King's College London
Jos GMEZ MARTNEZ	Universidad Autnoma de Madrid
Michael GAUS	Theoretical Chemistry, TU Braunschweig, Germany
Tamar GERSHON	Hebrew university
Matteo GUGLIELMI	Ecole Polytechnique Federale de Lausanne
Roland GUICHARD	MPIPKS
Matteo GUZZO	Universit Statale di Milano - Bicocca
Ralf HAMBACH	Ecole Polytechnique, Palaiseau, France
Keisuke HATADA	LNF-INFN
Nicole HELBIG	ETSF San Sebastian
Hannes HBENER	LSI, Ecole Polytechnique
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Lauri LEHTOVAARA	Helsinki University of Technology
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SeungKyu MIN	Pohang University of Science and Technology (POSTECH)
Petri MYHNEN	University of Jyvskyl
Mariana ODASHIMA	Universidade de So Paulo, Brazil
Roberto OLIVARES-AMAYA	Harvard University
Thomas OLSEN	Technical University of Denmark (DTU) - Physics
Max RAMIREZ	Universidad de Chile
Davide SANGALLI	Universit Degli Studi di Milano
Andr SCHLEIFE	Friedrich-Schiller-Universitt, Jena
Mireia SEGADO CENTELLAS	Universitat Rovira i Virgili
Alejandro SOBA	BSC
Lorenzo STELLA	University College London
Huub VAN DAM	STFC Daresbury Laboratory
Matthieu VERSTRAETE	Dept Phys University of York UK
Jos Guilherme VILHENA	Universite Lyon 1
Marius WANKO	BCCMS, University of Bremen
Ingolf WARNKE	University of California, Irvine
Joel YUEN	Harvard University
Martijn ZWIJNENBURG	Universitat de Barcelona

List of School Teachers

Xavier ANDRADE	Universidad del Pais Vasco
Silvana BOTTI	LSI Ecole Polytechnique
Manuel CARDONA	Max-Plack Stuttgart
Alberto CASTRO	Free University of Berlin
Marcus ELSTNER	Theoretical Chemistry, TU Braunschweig, Germany
Pablo GARCIA GONZALEZ	Universidad Nacional de Educacion a Distancia
Matteo GATTI	ETSF - LSI - Ecole Polytechnique
Rex GODBY	University of York
Hardy GROSS	Free Universitat Berlin
Conor HOGAN	Physics Department, University of Rome
Neepa MAITRA	Hunter College of the City University of New York
Andrea MARINI	Physics Department, University of Rome
Miguel MARQUES	LPMCN University Lyon 1
Fernando NOGUEIRA	CFC, University of Coimbra
Micael OLIVEIRA	University of Coimbra
Stefano OSSICINI	Universit di Modena e Reggo Emilia
Yann POUILLON	Universidad del Pas Vasco UPV/EHU
Angel RUBIO	UPV/EHU
Robert SEND	Universitaet Karlsruhe
Osamu SUGINO	ISSP, the University of Tokyo
Ivano TAVERNELLI	EPFL- Lausanne
Carsten ULLRICH	University of Missouri
Robert VAN LEEUWEN	University of Jyvskyl
Daniele VARSANO	Natl. Center S3 INFM-CNR, Modena , ITALY
Kazuhiro YABANA	Center for Computational Sciences, University of Tsukuba

List of Workshop Participants

(besides the students and teachers from the school)

Roi BAER	The Hebrew University of Jerusalem
Arjan BERGER	Ecole Polytechnique, Palaiseau, France
Kieron BURKE	Irvine, USA
Mark CASIDA	Universit Joseph Fourier (Grenoble I)
Massimiliano DI VENTRA	UC, San Diego
Nikos DOLTSINIS	Kings College, London
Jussi ENKOVAARA	CSC - Scientific Computing
Claudia FILIPPI	Universiteit Leiden, Instituut-Lorentz
Klaas GIESBERTZ	VU University
Andreas GOERLING	University of Erlangen-Nuremberg
Maria HELLGREN	Lund University

Dirk HOFMANN	University of Bayreuth, Germany
Kerstin HUMMER	Vienna University
Sohrab ISMAIL-BEIGI	Yale University
Thomas KOERZDOERFER	University of Bayreuth, Germany
Stephan KUMMEL	University of Bayreuth
Ester LIVSHITS	The Hebrew University of Jerusalem
Ilja MAKKONEN	University of Liverpool
Risto NIEMINEN	Helsinki University of Technology
Tapio T. RANTALA	Tampere University of Technology
John REHR	University of Washington
Dario ROCCA	University of California at Davis
Pina ROMANIELLO	Ecole Polytechnique, Palaiseau, France
Gianluca STEFANUCCI	Universita di Roma Tor Vergata
Lorenzo STELLA	University College London
Yasutami TAKADA	Institute for Solid State Physics, Univ. of Tokyo
Meta VAN FAASSEN	VU University
Troy VAN VOORHIS	MIT
Claudio VERDOZZI	Lund University, Sweden