



Catherine Werner
European Science Foundation
ESF Scientific Programme “Towards Atomistic Materials Design” (Psi-k)
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San Sebastián 12th September 2006

Dear Catherine;

I am sending you a summary of the expenses related to the organization of the 2nd International Workshop and School “Time Dependent Density-Functional Theory: Prospects and Applications” held in Benasque, Spain from the 27th of August to the 11th of September. The scientific report of the workshop, including all activities, programme and book of abstracts is also being sent as an attachment. This file will be sent to Walter Temmerman to be included in the next Psi-k newsletter.

The number of applications (above 180) surpassed all expectatives and, of course, the limit of 45 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 students (graduate and postgraduate) also did participate in the workshop held just after the 10 days of school. The total number of participants was 90 from all over the world (including 16 females; four as invited speakers/lectures). The distribution was:

	Organizers	Teachers	Students	Invited	Participants	School	Workshop
Australia	0	0	0	0	1	0	1
Austria	0	0	3	1	0	3	4
Belgium	0	1	1	1	0	2	3
Brazil	0	0	2	0	0	2	2
Chile	0	0	1	0	0	1	1
Finland	0	0	3	1	0	3	3
France	0	3	2	4	1	5	7
Germany	1	4	5	7	1	9	16
Holland	0	1	3	1	0	4	5
Iran	0	0	3	0	0	3	3
Israel	0	0	0	1	0	0	1
Italy	0	1	4	3	1	5	8
Japan	0	0	0	1	1	0	2
Mexico	0	0	2	0	1	2	3
Portugal	2	3	3	0	1	6	7
Spain	1	3	3	1	0	6	7
Sweden	0	0	2	0	0	2	2
Switzerland	0	0	0	2	0	0	2
UK	0	1	0	1	2	1	3
USA	0	1	6	3	1	7	10
TOTAL	4	18	43	27	10	61	90

We have allocated all the ESF/Psi-k support (9500 Euros) to cover all local expenses of graduate and postgraduate students attending both the school and workshop as well as providing a contribution to the travel expenses. The other participants as well as invited speakers were supported by other grants (the students covered by the NANOQUANTA Network of Excellence and by the Spanish Ministry of Science and Technology)

Time dependent Density-Functional Theory: Prospects and Applications

2nd International Workshop and School

2006, August 27 - September 11

A. Rubio (U. País Vasco, Centro Mixto CSIC-UPV/EHU and DIPC, Donostia; arubio@sc.ehu.es)
E.K.U. Gross (Freie Universitaet Berlin; hardy@physik.fu-berlin.de)
M.A.L. Marques (Universidade de Coimbra; marques@nautilus.fis.uc.pt)
F. Nogueira (Universidade de Coimbra and Centro de Física Computacional; fnog@teor.fis.uc.pt)

Location:

We organize this event at the "[Benasque Center for Science](http://www.benasque-center.com)", Benasque, Spain, from August 27, 2006 to September 10, 2006. Benasque is a beautiful town in the heart of the Pyrenees. The school will take place from August 27 (Day 0 -arrival of students for the school) to September 6, and the workshop will start September 6 (arrival of participants to the workshop) and finish on September 11 (departure of all participants). ([building and facilities](#)) E-Mail: benasque@ecm.ub.es

Scope	School 27th August-6th September	Workshop 6th-10th September	
	Program List of participants Auxiliary material	Program List of participants PDF's of the talks	
Practical information:	Accomodation	Travel	Tourism
	Weather	Pictures	Sports

[Check list of participants](#) (organisers only)

Registration

- [Application form](#)
- [Check your registration data](#) (for registered participants only)
- [Book and check your accomodation here](#)

Registration will be closed on the 1st of June 2006. **USA participants** can apply for [NFS support](#). There is also support available from the **Marie Curie Psi-k training** programme ([click here for more details](#))

NOTE ON TRAVEL:

The Center will organize free bus trips from Barcelona to Benasque (on August 27 and on September 6). Departure will take place at 15.00h from the main door of the Facultat de Físicaes, Univ. Barcelona, Diagonal 647 and will stop at the Airport of Barcelona at 15.30h (at the bus bays, between Terminal A and B). Return bus will be organized on September 7 and September 11, departing at 9 am from Benasque. The trip by bus takes 6h. You can reserve a seat when booking your accomodation above.

This scientific meeting has received financial support from the following institutions:



In particular, the distribution of the ESF-Psi-k contribution to this meeting was as follows:

Student	Nation of Residence	Psi-k support
Marques, Miguel	Portugal	800
Lein, Manfred	Germany	1000
Furche, Fillip	Germany	600
Botti, Silvana	France	800
Pouillon, Yann	Belgium	800
Maitra, Neepea	USA	1100
Jhala, Chirag	India	800
Prezzi, Deborah	Italy	800
Lopez-Lozano, Xochitl	Mexico	400
Lorenzen, Florian	Germany	800
Elliot, Peter	USA	300
Sahu, Bhagawan	India/Germany	400
Martinez, Jorge	Spain	600
Attacalite, Claudio	France	300
		TOTAL: 9500 Euros

The foundation “Benasque Center for Science”, where the meeting was held, has a proper record accounting of all the expenses charged to the ESF-contribution. The total cost of the event is summarized in the Table including the ESF contribution.

Concept	Expenses	Support			
		Spanish MCyT.	ESF	CECAM	Others
Organising Committee	5000	800	0.00	0.00	4200
Support to participants	42000	5200	9500	6000	21300
Local expenses, social events	5000	-	0.00	0	5000
TOTAL	52000	6000	9500	6000	30500

Let me know if you need any additional information. Thank you for your help and support.
Sincerely,



Prof. Angel Rubio
 (Co-organizer of the 2nd International Workshop and School “Time Dependent Density-Functional Theory: Prospects and Applications”
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Time dependent Density-Functional Theory: Prospects and Applications

2nd International School

Benasque, 27 August – 6 September 2006

Program

Day	Hour	Title	T/P
28/8	9:30 - 11:00	TDDFT I – Introduction (EG)	T
	11:30 - 13:00	TDDFT II - Linear Response Theory (EG)	
	15:00 - 18:30	Introduction to the practical classes (codes Octopus, Self, Abinit) (MM+AM+YP)	P
29/8	9:30 - 11:00	TDDFT as a tool in chemistry I (FF)	T
	11:30 - 13:00	TDDFT III - Strong Fields (EG)	
	15:00 - 18:30	Quantum Dots I (AC+MM+MO+FN)	P
30/8	9:30 - 11:00	Many-Body I – Introduction (RG)	T
	11:30 - 13:00	TDDFT as a tool in chemistry II (FF)	
	15:00 - 18:30	Quantum Dots II (AC+MM+MO+FN)	P
31/8	9:30 - 11:00	Many-Body II - GW and BSE (RG+LR)	T
	11:30 - 13:00	TDDFT IV - Keldish formalism (RvL)	
	15:00 - 18:30	Quantum Dots III (AC+MM+MO+FN)	P
1/9	9:30 - 11:00	Many-Body III - Many-Body vs TDDFT (LR)	T
	11:30 - 13:00	Propagation schemes (AC)	
	15:00 - 18:30	OCTOPUS I (FN+MO+MM+AC)	P
2/9	Free (excursion to be announced)		
3/9	9:30 - 11:00	TDDFT V - Advanced topics I (RvL)	T
	11:30 - 13:00	Models for time-dependent phenomena I (ML)	
	15:00 - 18:30	OCTOPUS II (FN+MO+MM+AC)	P
4/9	9:30 - 11:00	TDDFT VI - Advanced topics II (RvL)	T
	11:30 - 13:00	Models for time-dependent phenomena II (ML)	
	15:00 - 18:30	ABINIT+SELF I (AM+LW+MB+PG+SB+YP)	P
5/9	9:30 - 11:00	TDDFT as a tool in biophysics (AR+MM)	T
	11:30 - 13:00	Nonadiabatic electron dynamics in TDDFT I (CU)	
	15:00 - 18:30	ABINIT+SELF II (AM+LW+MB+PG+SB+YP)	P
6/9	9:30 - 11:00	Nonadiabatic electron dynamics in TDDFT II (CU)	T
	11:30 - 13:00	Challenges in TDDFT and Final remarks (AR)	

Theoretical classes:

	Lecturer	Title(s)
AC	Alberto Castro (FU Berlin, Germany)	Propagation schemes
AR	Angel Rubio (San Sebastian, Spain)	TDDFT as a tool in biophysics + Challenges in TDDFT
CU	Carsten Ullrich (Missouri, USA)	Nonadiabatic electron dynamics in TDDFT I, II
EG	E. K. U. Gross (FU Berlin, Germany)	TDDFT I, II, III
FF	Filipp Furche (Karlsruhe, Germany)	TDDFT as a tool in chemistry I, II
LR	Lucia Reining (Paris, France)	Many-Body II, III
ML	Manfred Lein (MPI Heidelberg)	Models for time-dependent phenomena I, II
MM	Miguel Marques (Coimbra, Portugal)	TDDFT as a tool in biophysics
RG	Rex W. Godby (York, UK)	Many-Body I, II
RvL	Robert van Leeuwen (Groningen, The Netherlands)	TDDFT IV, V, VI

Practical classes:

	Teacher	Session(s)
AC	Alberto Castro (FU Berlin, Germany)	QD, OCTOPUS
AM	Andrea Marini (Rome, Italy)	ABINIT+SELF
FN	Fernando Nogueira (Coimbra, Portugal)	QD, OCTOPUS
LW	Ludger Wirtz (Lille, France)	ABINIT+SELF
MB	Michel Bockstedte (San Sebastian, Spain)	ABINIT+SELF
MM	Miguel Marques (Coimbra, Portugal)	QD, OCTOPUS
MO	Micael Oliveira (Coimbra, Portugal and San Sebastian, Spain)	QD, OCTOPUS
PG	Pablo Garcia (Madrid, Spain)	ABINIT+SELF
SB	Silvana Botti (Paris, France)	ABINIT+SELF
YP	Yann Pouillon (Louvain-la-Neuve, Belgium)	ABINIT+SELF

Time dependent Density-Functional Theory: Prospects and Applications
2nd International Workshop
Benasque, 6 – 11 September 2006

Program

Day I: Thursday 7th		
09h00 - 09h10	Hardy Gross	Opening remarks
09h10 - 10h00	Neepta Maitra	Some challenges for time-dependent density functional approximations - and some partial solutions
10h00 - 10h50	N. Lathiotakis	Reduced density matrix functionals for finite and periodic systems
10h50 - 11h20	Caffeine break	
11h20 - 12h10	Mark Casida	Two-electron excitations in TDDFT
12h10 - 13h00	Stephan Kummel	Strong-field excitations and derivative discontinuities in TDDFT
13h00 - 15h00	Lunch break	
15h00 - 15h50	E. J. Baerends	Avoided crossings of excited state surfaces and vibronic coupling in TDDFT
15h50 - 16h40	Ivano Tavernelli	Non-adiabatic TDDFT MD: from gas phase to complex environments
16h40 - 17h10	Caffeine break	
17h10 - 18h00	Juerg Hutter	TDDFT calculations with the Gaussian augmented-plane wave approach
18h00 - 18h50	Rodolfo del Sole	Calculation of optical properties of complex systems within TDDFT
18h50 - 19h20	Dmitrij Rappoport	Practical aspects of molecular TDDFT calculations
Day II: Friday 8th		
09h10 - 10h00	Andreas Goerling	Exact exchange spin current density functional methods
10h00 - 10h50	Myrta Grüning	The effect of nonlocality on the band gap within density functional theory
10h50 - 11h20	Caffeine break	
11h20 - 12h10	Matteo Gatti	Nonlocality and frequency dependence of effective potentials
12h10 - 13h00	Rex Godby	Exchange-correlation functionals and kernels for conductance and polarization
13h00 - 15h00	Lunch break	
15h00 - 15h50	Massimiliano di Ventra	Transport in nanoscale systems: new approaches to an old problem
15h50 - 16h40	Gianluca Stefanucci	Time dependent transport phenomena within TDDFT
16h40 - 17h10	Beer break	
17h10 - 18h00	Carsten Ullrich	Time-dependent generating-coordinate method
18h00 - 20h00	Poster session, cheese and wine	
Day III: Saturday 9th		
09h10 - 10h00	Eckhard Pehlke	Molecular dynamics simulations of non-adiabatic processes
10h00 - 10h50	Roi Baer	Nonadiabatic functionals and their effects on electron dynamics in molecules and metal clusters
10h50 - 11h20	Caffeine break	
11h20 - 12h10	Esa Räsänen	Optimal laser control of quantum rings
12h10 - 13h00	Silvana Botti	How do rewritable DVDs work: optical properties of phase-change materials
13h00 - 15h00	Lunch break	
15h00 - 15h50	Ludger Wirtz	Electronic excitations in hexagonal layered systems (C and BN)
15h50 - 16h40	Deborah Prezzi	The role of excitons in the optical properties of carbon nanotubes
16h40 - 17h10	Beer break	
17h10 - 18h00	Marti Pi	TDDFT description of electronic systems in semiconductor heterostructures
18h00 - 19h30	Oral presentation of the best posters	
Day IV: Sunday 10th		
09h10 - 10h00	Stefano Baroni	Turbocharging time-dependent density-functional theory with Lanczos chains
10h00 - 10h50	Yoshi Miyamoto	TDDFT-MD simulation of nano-carbons: decay dynamics of hot-carriers and electronic shakeup by high-speed ions/atoms
10h50 - 11h20	Caffeine break	
11h20 - 12h10	Patrick Rinke	The band gap of InN and ScN: a quasiparticle energy study based on exact-exchange density-functional theory
12h10 - 13h00	C Ambrosch-Draxl	The role of core states on the excitation spectra of solids
13h00 - 13h20	Angel Rubio	Closing remarks