Research Networking Programmes

Science Meeting – Scientific Report

Scientific report (one single document in WORD or PDF file) should be submitted online within two months of the event. It should not exceed seven A4 pages.

***Proposal Title**:* 6th School and Workshop on Time Dependent Density Functional Theory: Prospects and Applications

Application Reference N°: 5195

1) Summary (up to one page)

This School & Workshop has been the sixth of a series that started in 2004 at the "Centro de Ciencias de Benasque Pedro Pascual" ("Pedro Pascual Center for Science at Benasque"), located in the village of Benasque, Spain. Following the successful scheme of previous years, we have had a School first, in which we have had a very intese introduction to the theory, practice, and numerical implementation of time-dependent density-functional theory (TDDFT). Then, we have had a Workshop, that has covered most of the main aspects surrounding TDDFT, discussed by the leading authors of the field.

2) Description of the scientific content of and discussions at the event (up to four pages)

Since TDDFT is a rapidly evolving field of Science, the precise content of both school and workshop have changed over the years – although the format of the events has been largely unaltered.

School

The School covered the topics that we believe constitute the core of the theory, and also included a few lectures about the experimental aspects that TDDFT intends to describe.

- Foundations of the theory, cornerstone theorems.

- Foundations of many-electron theory, which permits to study complementary theories for the description of many-electron dynamics: GW, Bethe-Salpether.
- Overview of spectroscopies: description of experiments, by leading experimentalists in the field.
- TDDFT approach to quantum electronic transport.
- Advanced concepts: memory, etc.
- Applications.

The theoretical work was complemented, in the afternoons, by practice work in the computer room of the Benasque Center for Science, where the students could access state-of-the-art software for TDDFT calculations. The practical work was divided in three sections:

- Software development: guided construction of a TDDFT code. The students had the opportunity of analyizing a basic TDDFT code, in order to develop skills in software engineering of this kind of programs.
- Tutorial on the octopus code.
- Tutorial on the BerkeleyGW code., including the interfase with octopus

Workshop

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:

- Fundamental topics on TDDFT, essential theorems.
- Femto- and atto-second dynamics of electrons in molecules and materials spin dynamics. Optimal control theory
- Many-Body Theory, and electron transport theory.
- New approximations to the exchange and correlation potential and kernel in density functional theory as well as density matrix theory
- Quantum optimal control.

- New experimental results, mainly in the areas of high intensity fields and atto-second Science.

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 members of other communities use the same techniques.

It is worth mentioning that the first day of the Workshop was largely occupied by speakers coming from the CRONOS EU project (www.cronostheory.eu).

The detailed program of both School and Workshop is given at the end of this document.

One-poster sessions were scheduled; the posters were hanged at the beginning of the event, and were kept at all times, so that students and participants could discuss at any time. In order to incentivate the creation of good posters, we organized a contest in which the four best posters (as qualified by a poll in which all School teachers could vote) got the ``Pedro Pascual Prize''. Those winners, who received equal number of votes, were invited to present their work at the Workshop. Those winners, along with the topic of their talks, were:

- Guillermo Albareda (Non-adiabatic dynamics)
- Tuomas Rossi (Quantum nanoplasmonics)
- Johannes Flick (Real time dynamics for QED)
- Yasumitsu Suzuki (Exact electron and nuclear TD-PES)

3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

The previous successes of this event is proved every time by the application numbers: In all occasions there has been a very large number of applicants for the school, that has increased every edition to become more than 100. This is not only a testimony of the strong pulse of the scientific field itself, but also of the good quality of the school. Since we want to maximize the learning experience of the students via a close interaction with the teachers (and also due to the logistic limitations imposed by the hands-on tutorial), the participants of the school have never exceeded 50. It is worth mentioning that participants came from all over the world, making this series of schools and workshops a truly global event.

The work presented at the Workshop has demonstrated the outstanding capabilities of TDDFT to describe the various forms of spectroscopy that probe the electron dynamics of matter. Spectroscopies, in general, are the tools used to study the microscopic structure of matter. The experimental results obtained with these tools can only be interpreted correctly with the help of accurate theoretical methods, capable of simulating the microscopic behavior of matter subject to external perturbations. A number of spectroscopic methods address electronic excited states (e.g. optical absorption spectroscopy, photo-electron emission spectroscopy, etc), and hence the needs of first principles theoretical methods capable of addressing the excited state many-electron problem. Time-dependent density-functional theory (TDDFT) is one of such methods.

It is not, however, the only approach to the excitations of many-electron systems. In fact, more accurate (yet more expensive) techniques (based on many-body perturbation theory, for example) exist, and therefore these alternatives have also been covered in both the workshop and the school – in particular their relation and comparison to TDDFT. However, TDDFT achieves a good balance between accuracy and computational cost. This workshop has clearly shown how its use is increasing, and it is fast becoming one of the tools of choice to get accurate and reliable predictions for excited-state properties in solid state physics, chemistry and biophysics, both in the linear and non-linear regimes.

We have witnessed in this Workshop the most recent developments of TDDFT (and time-dependent current functional theory): the description of photo-absorption cross section of molecules and nanostructures, electron-ion dynamics in the excited state triggered by either a small or high intense laser fields, van der Waals interactions, development of new functionals coping with memory and non-locality effects, applications to biological systems (chromophores), transport phenomena, optical spectra of solids and low-dimensional structures (as nanotubes, polymers, surfaces...).

The scientists that approach the TDDFT field face difficulties in grasping its many aspects, and we feel that for those attending the School, these difficulties have been alleviated. We believe that the School has been extremely helpful for young graduate students, post-docs that are envisaging a project for which TDDFT/MBT is the tool of choice. The event is especially useful, since we feel that the most efficient scheme for training young researchers in these techniques is to have a school where the basic theory is taught, followed by a workshop that introduces them to the forefront research in the field. The school had an equal share of theoretical and practical classes. This eases the learning of the techniques and provides the students with the practical knowledge of the numerical aspects and difficulties, at the same time introducing them to well-established open source numerical codes. At the end of the School, the students have reached sufficient working knowledge to pursue their projects at their home institution.

During the school we have incentivated a close and informal contact between the students and the teachers. Furthermore, the students had the opportunity of talking about their current research activities and future interests. We feel that this is an important point, since young scientists should be involved in the building up of a strong community.

Finally, we mention that, as in other editions of this event, we made a survey among all participants in order to assess the level of satisfaction. We can report that in general we received a very positive feedback. Most participants found both Workshop and School to be most stimulating, even more than in past editions.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

Sunday, January 05

- 09:30h DFT I
  Kieron Burke

- 10:30h DFT II
  Kieron Burke
- 11:30h TDDFT I
  E. K. U. Gross
- 12:30h TDDFT II
  E. K. U. Gross
- 15:30h Introduction to coding for electronic structure modeling

Monday, January 06

- 09:30h DFT III
  Kieron Burke
- 10:30h TDDFT III
  E. K. U. Gross
- 11:30h Introduction to Many Body Theory I
  Robert van Leeuewn
- 12:30h Introduction to Many Body Theory II
  Robert van Leeuwen
- 15:30h Introduction to coding for electronic structure modeling

Tuesday, January 07

- 09:30h DFT IV
  Kieron Burke
- 10:30h Introduction to Many Body Theory III
  Robert van Leeuwen
- 11:30h TDDFT Advanced Topics I
  Neepa Maitra
- 12:30h TDDFT Advanced Topics II
  Neepa Maitra
- 15:30h Tutorial: octopus code

Wednesday, January 08

- 15:30h Tutorial: octopus code

Thursday, January 09

- 09:30h Non-linear response in TDDFT
  David Strubbe
- 10:30h Q&A session - TDDFT
  Hardy, Kieron, Robert, Neepa
- 11:30h Q&A session - TDDFT
  Hardy, Kieron, Robert, Neepa
- 12:30h Q&A session - TDDFT
  Hardy, Kieron, Robert, Neepa
- 15:30h Practical: octopus

Friday, January 10

- 15:30h GW I
  Matteo Gatti
- 16:30h GW II
  Matteo Gatti
- 17:30h TDDFT for Chemists I
  Ivano Tavernelli
- 18:30h TDDFT for Chemists II

Ivano Tavernelli

Saturday, January 11

- 09:30h Bethe-Salpeter I
  Ilya Tokatly
- 10:30h Bethe-Salpeter II
  Ilya Tokatly
- 11:30h TDDFT + Molecular Dynamics I
  Ivano Tavernelli
- 12:30h Spectroscopy from an experimentalist's viewpoint I
  Simo Huotari
- 15:30h Tutorial: BerkeleyGW

Sunday, January 12

- 09:30h TDDFT + Molecular Dynamics II
  Ivano Tavernelli
- 10:30h Spectroscopy from an experimentalist's viewpoint II
  Simo Huotari
- 11:30h Nonperturbative quantum dynamics I
  Manfred Lein
- 12:30h Q&A session MBPT
- 15:30h Tutorial: BerkeleyGW

Monday, January 13

- 09:30h Non perturbative quantum dynamics II
  Manfred Lein
- 10:30h Molecular Electronics I
  Stefan Kurth
- 11:30h Molecular Electronics II
  Stefan Kurth
- 12:30h Open session about challenges and standing problems
  Angel Rubio

Tuesday, January 14

- 09:45h Real-time spin dynamics in TDDFT
  Stefano Sanvito
- 10:15h Electronic properties of artificial graphene
  Esa Räsänen
- 10:45h Time-resolved spectroscopies for atoms and molecules with TDDFT
  Umberto de Giovanninni
- 12:00h Coupled electron-nuclear dynamics beyond the Born-Oppenheimer approximation
  Hardy Gross
- 12:30h On non-collinear gradient expansions and their generalizations in spin-density-functional theory
  Stefano Pittalis
- 15:30h Ultrafast dynamics of exciton formation and relaxation at the ZnO(10-10) surface
  Julia Stähler
- 16:00h Charge-to-current conversion in artificial light harvesting systems and organic solar cells: Ultrafast spectroscopy and TDDFT simulations
  Antonietta de Sio

- 17:00h Probing magnetic phenomena of single molecules on metal and superconducting surfaces
  Nacho Pascual
- 17:30h Inelastic x-ray scattering: recent applications
  Simo Huotari
- 18:00h Dye Sensitized Solar Cell Progress
  Toby Meyer
- 18:30h POSTER SESSION

Wednesday, January 15

- 16:00h TDDFT for many-body systems driven by a quantized electro-magnetic field
  Ilya Tokatly
- 16:30h Real-time evolution of correlated photon-electron wavefunctions in quantum electrodynamics
  Heiko Appel
- 17:00h Poster Prize Talk: Real-time propagations for correlated systems in Fock space
  Johannes Flick
- 17:45h TBA
  Garnet Chan
- 18:15h Excited-state forces in TDDFT and the Bethe-Salpeter equation
  David Strubbe
- 18:45h Tuning the photophysics of biological chromophores
  Marius Wanko

Thursday, January 16

- 09:30h Dynamical exchange-correlation corrections to transport
  Stefan Kurth
- 10:00h Ultra-nonlocality in density-functional theory for photo- emission spectroscopy
  Robert van Leeuwen
- 10:30h First-principles calculations of spectral functions: spin multiplets, plasmon satellites, and spin fluctuations
  Johannes Lischner
- 11:45h Stochastic methods for gentle scaling of electronic structure methods with acronyms we love and trust (DFT, MP2, RPA, GW)
  Roi Baer
- 12:15h Time-dependent natural orbital theory applied to worst-case TDDFT problems”
  Dieter Bauer
- 12:45h Dissipative effects in quantum time dependent mean field
  Eric Suraud
- 13:15h LUNCH

- 16:00h Poster Prize Talk: Non-Adiabatic dynamics with the conditional wave functions
  Guillermo Albareda
- 16:20h Poster Pize Talk: Exact electronic and nuclear time-dependent potential energy surface for attosecond electron localization in the dissociation H2+
  Yasumitsu Suzuki
- 16:40h Time-dependent DFT and time-dependent tight-binding: Opportunities and Challenges
  Mathias Nest
- 17:10h Electronic structure methods based on the adiabatic- connection fluctuation-dissipation theorem
  Andreas Görling

Friday, January 17

- 09:00h Materials design using real-time TDDFT: from clusters to proteins
  Micael Oliveira
- 09:30h Poster Prize Talk: Atomistic approach for the field enhancement in quantum plasmonics nanostructures
  Tuomas Rossi

- 10:30h Frenkel versus charge-transfer exciton dispersion in molecular crystals
  Pierluigi Cudazzo
- 11:00h Dressed TDA-TDDFT approach to doubly-excited configurations
  Grzegorz Mazur
- 11:30h Closing Remarks and next Benasque meeting in 2016
  The Organisers

Annex 4b: Full list of speakers and participants

SCHOOL TEACHERS (some of them are also speakers at the Workshop)
Kieron Burke
Robert van Leeuwen
Matteo Gatti
David Strubbe
Ivano Tavernelli
Ilya Tokatly
Simo Huotari
Manfred Lein
Stefan Kurth
Micael Oliveira
Felipe Homrich da Jornada
INVITED SPEAKERS
Stefano Sanvito
Esa Räsänen
Umberto de Giovanninni
Stefano Pittalis
Julia Stähler
Antonietta de Sio
Nacho Pascual
Toby Meyer
Pierluigi Cudazzo
Andreas Görling
Garnet Chan
Matthias Nest
Heiko Appel
Marius Wanko
Roi Baer
Dieter Bauer
Eric Suraud
Grzegorz Mazur
Johannes Lischner
PARTICIPANTS OF THE WORKSHOP ONLY
Ali Abedi
Mohammed Attrash
Arkadiy Davydov
José María Escartín
Mehdi Farzanehpour
Johannes Flick
Johanna Fuks
Nicole Helbig
Per Hyldgaard
Jeiran Jokar
Joaquim Jornet Somoza
Ask Hjorth Larsen
Di Liu
Seung Kyu Min
Victor Morón
Dario Rocca
Carlo Rozzi

Iris Theophilou
Jessica Walkenhorst
Xian Lede
Christoph Lienau
SCHOOL STUDENTS
Attrash, Mohammed
Guillermo Albareda
Enrico Berardo
Robert Biele
Jorge Budagosky
Gloria Capano
Sophie Chauvin
Alain Delgado Gran
Victor Despré
Stefano di Sabatino
Tanjia Dimitrov
Greta Donati
Felipe Franco de Carvalho
Livia Noemi Glanzmann
Beatriz González del Rio
Pierre Guiglion
Rebecca Haddad
Marie Humbert-Droz
Alexander Hupfer
Daniel Jensen
Rene Jestadt
Elham Khosravi
Giovanna Lani
Irina Lebedeva
Kai Luo
Martin Madel
Juan Pablo Martínez
Yu-ichiro Matsushita
Paulo V. C. Medeiros
Rodrigo Migotto Seraide
Martín Mosquera Tabares
Jonathan Nafziger
Francesca Pecatti
Camilla Pellegrini
Yang Peng
Nathaniel Raimbault
Valerio Rizzi
Tuomas Rossi
Rafael Alejandro Sarmiento Pérez
Shunsuke Sato
Ravindra Shinde
Yasushi Shinohara
Nikolay Shvetsov-Shilovskiy
Fernando Silva
Jacopo Simoni
Adrián Soto
Yasumitsu Suzuki
Peter Thayer
Bruno Torcal-Embeita
Rafi Ullah
Alejandro Varas
Phillip Wopperer
Kaike Yang