PsiK report on the

8th School and Workshop on Time-Dependent Density-Functional Theory: Prospects and Applications

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Benasque Center for Science "Pedro Pascual", Benasque, Spain

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There are many alternative schemes to approach the time-dependent, out-of-equilibrium, many-electron problem. Time-dependent density-functional theory (TDDFT) has a significant "market share" due to the same reasons that make conventional ground state density-functional theory (DFT) a successful scheme: the fairly good predictive power at a moderate computational cost. As a consequence, its use has quickly grown, and its reliability for many purposes has been sanctioned by many applications and benchmarks over the years. As the computational resources increase, however, various alternatives such as advanced post-Hartree Fock multi-configuration schemes or many-body perturbation theory techniques can be applied to larger systems, and may provide more precise results. Newer and more intriguing possibilities, such as the direct solution of the many-electron Schrödinger equation with quantum computers, and the use of machine learning techniques for the prediction of many properties, appear also in the horizon. It is therefore necessary to review the capabilities and perspectives of TDDFT. This is the main goal of the Workshop, and of the School that we organized immediately before the Workshop.

This School+Workshop event is in fact a new iteration of a series dedicated to TDDFT, that started in 2004. It takes place every two years, a periodicity that we feel that is adequate to follow the advances in the topic. However, it always takes place in Europe, and there was a strong demand for a similar event taking place in the US, due to the difficulties in the travel, specially for students and young researchers. Fortunately, the demand was met in the last year by a similar event (a school on TDDFT followed by a workshop on first principles approaches to the electronic excited states problem) that took place in Telluride, Colorado. Part of the

organizers of this event were also present in Benasque, and the goal is to periodically repeat the US event, also every two years if possible. It should be noted, also, that a similar event is being planned in Asia (Tsukuba, Japan), by Prof. K. Yabana.

In this 2018 edition, we had a total attendance of 65 people, including 31 students during the School (the rest are school lecturers, invited speakers, and contributors for the Workshop). In addition to the scientific program, the outstanding location of the event permits the participants to enjoy the beauty of the valley of Benasque. Two mornings and one full day were free of scientific activity, and most participants used the opportunity to hike and/or relax in the mountains. The social program was complete with a workshop dinner the last day of the event.

SCHOOL

The program for both School and Workshop (as well as the list of participants) may be consulted at:

http://www.benasque.org/2018tddft/

As it can be learnt from it, the main topics of the School were

1. The fundamentals of DFT and TDDFT.
2. Many-Body Theory approaches to the problem of the electronic ground state and electronic excitations.
3. Review of the possible applications of DFT and TDDFT in physics and chemistry.
4. Non-linear processes: applicability of TDDFT to strong perturbations.
5. Numerics.
6. Advanced topics: the molecular Berry phase, topological invariants.

In addition, six hands-on session were used to initiate the students on TDDFT-based and many-body calculations (GW and Bethe-Salpeter). One poster session was held during the School (another one was held during the Workshop), and the lecturers voted for one outstanding poster (authored by Fumiyuki Ihii), who was given the opportunity of presenting his work at the Workshop.

There was a strong demand for the school (more than 80 applications). We has a positive feedback from the students (anonymous surveys were distributed). It should be noted that, with a few exceptions, all students participated also in the Workshop (they are strongly encouraged to do so).

The School material (slides, handouts for the hands-on sessions) can be downloaded from the event webpage.

SOME OF THE TOPICS DISCUSSED DURING THE WORKSHOP

We have witnessed in this Workshop (1) talks dedicated to the theretical foundations of TDDFT and its possible extensions; (2) talks dedicated to applications of TDDFT; (3) talks dedicated to alternatives to TDDFT; and (4) methodological topics.

The first session was entirely dedicated to the first of these groups: Ilya Tokatly discussed the combination of TDDFT with the quantum-mechanical treatment of the photon field, in order to address cavity quantum electrodynamics problems, whereas Carsten Ullrich presented research on the exchange-and-correlation functional – always the key fundamental problem of TDDFT. In a later session, Eric Suraud summarized theoretical results about the inclusion of dissipative effects in TDDFT. A very different theoretical problem was addressed by Ryan Requist: the issue of separating the electronic and nuclear wave function, typically handled by the Born-Oppenheimer approximation, can also be treated within an “exact” factorization scheme pioneered by Hardy Gross and collaborators in recent years within the TDDFT context. Ryan Requist presented new research, focusing on the approximation of the necessary functionals. Roi Baer also addressed a theoretical topic: a stochastic approach for evolving in real time non-interacting Fermions in open quantum systems under the influence of a bath. Finally, the work presented by Emmanuel Fromager also belongs to the group of theoretical developments: the use of DFT for ensembles in order to study the fundamental and optical gaps.

Various talks were dedicated to the second group mentioned above: applications of TDDFT. It became apparent, therefore, the wide applicability range of TDDFT, and how it can be used to approach non-equilibrium problems. Various examples were displayed: (1) the calculation of optical spectra of dyes in solution presented by Christine Isborn, who showed how solvent effects can be taken into acount; (2) the calculation of high-harmonic generation spectra from solids shown by Nicolas Tancogne-Dejean; (3) various applications of TDDFT in the realm of attosecond physics, summarized by Shunsuke Sato, (4) a review of the capabilities and shortcomings of TDDFT for the description of optical properties of materials, provided by Arjan Berger; (5) a discussion on the ability of TDDFT to describe non-linear optical properties of solids by Valerie Veniard; and (6) the problem of proton stopping power of materials, reviewed by André Schleife.

All previous talks centered on applications of TDDFT were good opportunities to discuss the shortcomings of the theory, whose origin is traced to the lack of a good approximation to the exchange and correlation potential, or to the lack of good approximations to some of the observables. Therefore, it is necessary to establish comparisons with other theories. Some examples: density functional perturbation theory from constrained DFT (David Strubbe), time-dependent two-particle density matrix theory (Joaquim Burgdörfer), the calculation of the spectral function from steady-state DFT (Stefan Kurth), reduced density matrix functional theory (Carlos Benavides-Riveros). But perhaps the most intriguing approach was the use of quantum computation techniques for the solution of highly correlated quantum-chemistry methods, described by Ivano Tavernelli. Although at an early stage both from the theoretical, software, and hardware perspectives, this scheme may be a revolutionary approach to the quantum chemical problem.

Finally, some time was dedicated to methodological advances: for example, Adrián Gómez Pueyo presented research on propagators for the TDDFT equations, and Peter Koval discussed the use of numerical atomic orbitals. We also emphasize that a younger generation of scientists was present, since most of the students of the school stay for the ensuing workshop. The students had the occasion of showing their research during a poster session, and one of them (Fumiyuki Ishii), selected by a vote, could present a talk.