17th ETSF Workshop on electronic excitations (ETSF2012)

Combra Portugal 1/10 to 6/10 2012

Funding CECAM, Psi-k, ESF and UCoimbra

Claudio Attaccalite, Myrta Grüning, Fernando Nogueira, Nicole Helbig, and Matthieu Verstraete

http://www.tddft.org/ETSF2012/

0.1 Summary

The 2012 ETSF workshop on excited electronic states was an overview of the state of the art in the Green's function methods which are the core business of the ETSF since its inception. Particular attention was paid to recent efforts to assess quantitatively the accuracy of different methods, most importantly the starting electronic structure we obtain from density functional theory. As in previous years, prominent experimentalists were invited to present their latest results in the fields of spectroscopy and ultrafast electron and ion dynamics - these are precious interactions guaranteeing the synchronicity of theoretical and experimental efforts for the future. Invited and contributed talks were divided thematically, each session being initiated by an invited or highlighted talk with an overview and perspective on the sub-field and more time for questions. Finally, the last half-day was devoted to a collaborative session with the PRACE initiative, featuring important overviews of coming technologies in supercomputing and case studies of electronic structure code performance on cutting-edge HPC machines.

The conference venue in Coimbra was a very agreeable and efficient one, in the setting of one of the oldest universities in the world, where we were able to access extensive infrastructure for lecture halls and internet access, and organize efficiently the transport of participants, catering, and accommodation details.

The annual conference is also an important venue for organization between members of the growing European Theoretical Spectroscopy Facility. Steering committee and working group meetings were held before and after the conference. The new scientific steering committee elected a chair and vice-chair, and progress was made made in structuring the user-service functions of the ETSF. The different themed collaboration teams also echo specific preoccupations of Psi-k: electron correlation, electron-vibration coupling, and the simulation of large and/or biological systems. Several of the teams continuously submit workshop proposals to Psi-k, and benefit from the ETSF workshop to plan these and other future proposals.

Conclusion

The ETSF 2012 conference was a very successful edition, both through the rich interactions and the high quality of the invited speakers which were attracted. Students benefitted extensively from the talks and informal discussions during coffee breaks, obtaining a systematic overview of the field of spectroscopy, both for cutting edge experimental techniques and the latest theoretical developments. The conference in this form was only possible thanks to vital sources of conference-specific funding provided by Psi-k, the ESF, the University of Coimbra, the PRACE supercomputing network, and CECAM. The low conference fee and additional bursaries for students was particularly welcome in the present context of wide budget cuts in science and travel funding in particular. Researchers from the USA, Italy, but also France and Spain would not have been able to come without the basic financial support provided to the conference. We look forward to continuing the ETSF conference series - the next edition will be at the University of Luxembourg, and focus on the contribution

of excited states and spectroscopic techniques to the development of energy materials: thermoelectrics, photovoltaics, and functional oxides and alloys.

0.2 Scientific content and discussions

In the following, the main themes of the presentations are summarized, along with salient contributions from invited speakers.

Time resolved spectroscopies

Femto and attosecond laser pulses are now engineered routinely in experiments on ultrafast chemistry and physics, probing and stimulating electron and nuclear dynamics on the shortest possible time scales. These systems remain extremely challenging experimentally, and were presented by Mark Vrakking (MBI Berlin), representing the different timescales of (respectively) vibrational and purely electronic phenomena. This area of spectroscopy has seen a huge increase in theoretical investment in the past 5-10 years, which has been tracked by the development of the corresponding beamline in the ETSF. Theoretical models to treat real-time and ultrafast dynamics were presented by Jun Haruyama (Tokyo U Science) Kay Dewhurst (MPI Halle) and Theodoros Papadopoulos (U Liege), covering both advances in time dependent density functional theory and non-adiabatic time evolution.

Systematic assessment and development of theoretical accuracies

The assessment of accuracies in numerical methods is often very complex, and many quantities are uncontrolled. Recently Prof Stefaan Cottenier (U Ghent) has begun benchmarking competing theoretical programs to evaluate the absolute accuracies they provide, with respect to each other and with respect to experimental "truth". Improved methods for large systems and the calculation of total energies and band structures within the GW approximation were described by Prof Feliciano Giustino (U Oxford). The systematic improvement of GW calculations for strongly correlated systems is an ongoing challenge in our field, which has been developed forcefully by Prof Aryasetyawan (U Lund) over the past 10 years - his presentation on the latest ab initio methods to calculate Hubbard parameters and to use dynamical mean field theory in combination with GW were an excellent summary of the state of the art at present.

Photoemission spectroscopy

The theoretical prediction of angle resolved photoemission experiments is quite complex, and an important new step has been demonstrated by Umberto De Giovannini (U Pais Vasco San Sebastian) using time dependent DFT. These techniques are linked to common work in the fields of Prof Zyss (EN Cachan) in non-linear spectroscopy and Prof Vrakking (MBI Berlin) in ultrafast spectroscopy.

PRACE session

Most of the calculations of electronic structure on challenging systems require large amounts of computer power, and usually entail parallel computations on many tens, hundreds, and now thousands of processors. PRACE is the central European entity managing the collaborative network of scientific computing centers, their development and their evolution. The continuous adaptation of our computing programs to the specific and complex architectures of PRACE machines is a full-time job, and regular interaction and interfacing with PRACE engineers is crucial to all researchers in ab initio techniques. We have been very

fortunate this year to have a joint conference session with PRACE, and the presentation of both technical overviews and perspectives on HPC in the future (Drs Girotto and Affinito) and a number of case studies by ETSF scientists (in particular Dr Giantomassi) who are at the forefront of our field in exploiting fully the HPC resources at PRACE computing centers.

0.3 Results and impact on future of the field

The ongoing series of ETSF conferences (for over 15 years) have been fundamental in structuring the field of electronic excited states, in particular they popularized the denomination of "theoretical spectroscopy" which is now used extensively by other groups and conferences in the Psi-k and DFT communities.

The impact of the 2012 edition will be felt in the widening of the theoretical spectroscopy community and in strong progress in identifying and addressing key challenges in the field. A clear need for expanding the scope of the present conference and opening and advertising it to the whole community has become self-evident, and will be addressed by the size and outreach of the 2013 edition, whose organization is already well under way. The challenges addressed by the different sessions in 2012 point clearly to the types of systems and methods which will have to be addressed in the coming years: coherent treatments of strongly and "normally" correlated electrons, large systems with hundreds of atoms and requiring extensive computing infrastructure, and the treatment of time-dependent (often ultrafast) phenomena. The current and future workshops represent the most important computational packages and codes (quantum-espresso, SIESTA, Fleur, ABINIT, OCTOPUS, FHI-Aims, VASP and others), but also communities, going from strongly correlated systems to quantum chemistry, with a strong showing of many-body perturbation theory. The conference is a vital terrain for confrontation and validation of different approaches, implementations, and the discovery of novel systems and algorithms.

0.4 Program

Tuesday 2 October
Registration and Opening
Error bars for solid-state density-functional theory predictions *Stefaan Cottenier*
Ground-state properties from Many-Body Perturbation Theory: is self-consistent GW good enough? *Fabio Caruso*
Validation of calculations based on electron-phonon matrix elements in Abinit and PWSCF/Yambo/EPW *Samuel Poncé*
Pragmatic band gap calculations as a "sieve" for experimental tabulations *Daria M. Tomecka*
Assessment of electronic band structure from the Tran-Blaha functional : comparison with Many-Body Perturbation Theory results *David Waroquiers*
Simulation of electronic transport in defective graphene. From point defects to amorphous structures. *Aurélien Lherbier*

PM
Bridging density-functional and many-body perturbation theory: orbital-density dependence in electronic-structure functionals *Andrea Ferretti*
Resonant Electron Tunneling - Exact vs. DFT Description *Jessica Walkenhorst*
Ab-initio Description of Satellites in Semiconductors *Matteo Guzzo*
Role of non-local exchange in the electronic structure of correlated oxides *Federico Iori*
Dynamical effects in electronic excitations of carbon based nanostructures *Lorenzo Sponza*
Exciton dispersion in wide-gap insulators: there and back again *Francesco Sottile*
Poster Session

Wednesday 3 October
Multi-material and multi-functional developments in Nonlinear Optics down to the nanoscale *Joseph Zyss*
Second order harmonic generation in bulk semiconductors and nanostructures. *Valérie Véniard*
Non-adiabatic effects within a single thermally-averaged potential energy surface: Thermal expansion and reaction rates of small molecules *Alberto Castro*
Molecular dynamics simulation of biphenyl under strong laser pulses: a TDDFT investigation *Jun Haruyama*
Insights into the surface hopping approach from a wave packet limit *José María Escartín*
Time-Dependent Density Functional Theory study of charge transfer in collisions *Guillermo Avendaño-Franco*

PM
Conductance of organic molecules and graphene derived systems with graphene

leads *Brivio Gian Paolo*
Nanoplasmonics response of graphene-like systems by Time-Dependent Density-Functional Theory *Fulvio Berardi*
Electronic excitations in thin-film absorbers for photovoltaics *Silvana Botti*
Excitons in molecular solids: picene vs pentacene *Pierluigi Cudazzo*
Identifying cationic positoins within zeolites - Modelling the absorption spectra of Cu(I) sites in chabazite *Florian Goeltl*
Electronic and optical properties of CdF2 and BaF2: The role of many-body effects *Juergen Furthmueller*
Dynamical response of layered transition-metal dichalcogenides: ab initio microscopic analysis of the plasmon dispersion *Matteo Gatti*
ETSF general meeting

Thursday 4 October
Attosecond Time-Resolved Molecular Dynamics *Mark Vrakking*
Real-time evolution in solids on the attosecond time scale *John Kay Dewhurst*
Control of electron density dynamics; from small to larger organic molecules *Theodoros A. Papadopoulos*
Nonequilibrium Green function approach to ultrafast electronic dynamics in molecular systems *Adrian Stan*
Rydberg series of excitons: dynamical bootstrap approximation for the kernel of time-dependent density functional theory *Sangeeta Sharma*
Determination of the one-body Green's function: freedom and constraints *Pina Romaniello*

PM
Effective Coulomb Interaction of Many-Electron Systems *Ferdi Aryasetiawan*
RPA model for interatomic many-body van der Waals interactions *Alberto Ambrosetti*
Renormalized second-oder perturbation theory for the electron correlation energy: concepts and benchmarks *Patrick Rinke*
Ab-initio angle and energy resolved photoelectron spectroscopy with time-dependent density-functional theory *Umberto De Giovannini*
Spectroscopy of TiO2 and HfO2 polymorphs *Linda Hung*
Electronic Excitations in CuO: Quasiparticles and Satellites *Claudia Rödl*
Technical and Administrative meetings

Friday 5 October
GW quasiparticle calculations using the self-consistent Sternheimer equation *Feliciano Giustino*
Extension of an O(N3) implementation of Hedin's GW method from clusters to periodic crystals *Dietrich Foerster*
Speeding up the solution of the Bethe-Salpeter equation by a double-grid method and Wannier interpolation *David Kammerlander*
The GW Method for Quantum Chemistry applications: Theory, Implementation, Benchmarks *Michiel J. van Setten*

High-throughput ab initio computations for materials discovery and the Materials Project database *Geoffroy Hautier*
Role of oxidation in the yellowing of Leonardo Da Vinci's self-portrait *Adriano Mosca Conte*

PM : PRACE presentations
Accelerated QE-PWscf code for hybrid system equipped with NVIDIA GPU: development experience and performance analysis *Ivan Girotto*
Bluegene/Q for material science. First experiences with FERMI *Fabio Affinito*
High performance computing with Abinit and Bigdft: performance analysis and code refactoring within the PRACE project *Matteo Giantomassi*
Closing Remarks

Participant list

Amato Michele
Affinito Fabio
Ambrosetti Alberto
Aryasetiawan Ferdi
Attaccalite Claudio
Avendaño-Franco Guillermo
Berardi Fulvio
Beuken Jean-Michel
Botello Andres
Botti Silvana
Brivio Gian
Bruant Gaelle
Caruso Fabio
Castañeda Arcesio
Castro Alberto
Charlier Jean-Christophe
Chibani Wael
Cottenier Stefaan
Cucca Andrea
Cudazzo Pierluigi
Da Pieve Fabiana
De Giovannini Umberto
Declerck Xavier
Dewhurst John Kay
Di Gennaro Marco
Escartín José María
Ferretti Andrea
Foerster Dietrich
Fratesi Guido
Furthmueller Juergen

Garcia-Gonzalez Pablo
Gatti Matteo
Giantomassi Matteo
Gillet Yannick
Giorgetti Christine
Girotto Ivan
Giustino Feliciano
Godby Rex
Goeltl Florian
Gonze Xavier
Grüning Myrta
Guzzo Matteo
Haruyama Jun
Hautier Geoffroy
Helbig Nicole
Hogan Connor
Hung Linda
Iacomino Amilcare
Ibarra Wilfredo
Iori Federico
Kammerlander David
Kostov Gueorguiev Gueorgui
Leconte Nicolas
Lherbier Aurélien
Lora Estelina
Malcioglu Baris
Marini Andrea
Marques Miguel A.L.
Miglio anna
Milne Bruce
Molinari Elisa
Molina-Sánchez Alejandro
Mosca Conte Adriano
Nemec Lydia
Nicolaev Adela
Nogueira Fernando
Olevano Valerio
Oliveira Micael
Onida giovanni
Paixão José António
Papadopoulos Theodoros A
Poncé Samuel
Pouillon Yann
Rehr John J
Reining Lucia
Rignanese Gian-Marco

Rinke Patrick
Rödl Claudia
Romaniello Pina
Rozzi Carlo Andrea
Sharma Sangeeta
Sidónio Pedro
Sottile Francesco
Sponza Lorenzo
Stan Adrian
Tancogne-Dejean Nicolas
Tandetzky Falk
Thrupp Nicola
Tomecka Daria M
Van Setten Michiel
Véniard Valérie
Verdozzi Claudio
Verstraete Matthieu
Violante Claudia
Virk Kuljit
Vlcek Vojtech
Vrakking Mark
Walkenhorst Jessica
Waroquiers David
Werner Ute
Zisser Wolfhard H
Zyss Joseph