17th ETSF Workshop on electronic excitations
(ETSF2012)
Combra Portugal 1/10 to 6/10 2012
Funding CECAM, Psi-k, ESF and UCoimbra
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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 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 Cotte
nier

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: com-
parison 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 sur-
face: 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 colli-
sions Guillermo Avendaño-Franco

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Conductance of organic molecules and graphene derived systems with graphene
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 positons 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

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

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Effective Coulomb Interaction of Many-Electron Systems 
Ferdi Aryasetiawan

RPA model for interatomic many-body van der Waals interactions 
Alberto Ambrosetti

Renormalized second-order 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  
Attacalite 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
Giantomassì Matteo
Gillet Yannick
Giorgetti Christine
Girotto Ivan
Giustino Feliciano
Godby Rex
Goeltl Florian
Gonze Xavier
Grüning Myrta
Guzzo Matteo
Haruyama Jun
Hautier Geoffroy
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Migliö Anna
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