2.1.2 16th ETSF Workshop on electronic excitations (ETSF2011)

Turin Italy

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CECAM, Psi-k, ESF, and MaiMosine

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http://www.tddft.org/ETSF2011/

Report

The 2011 ETSF conference was centered on building bridges between theorists and experimentalists in our key fields, namely time-resolved, X-Ray, photoemission, optical, and other spectroscopies. The conference was constructed around the different types of techniques, with one or two invited talks by prominent experimentalists, followed by theoretical contributed (and a few invited) talks. A few additional sessions were added to account for methodological and fundamental developments, but these were kept to a minimum in the 2011 instance of the conference. Overall the interaction was very efficient, featuring both the development of collaborations between theoreticians on excited states in electron systems, which is the hallmark of the ETSF network, and also between experimentalists and theoreticians. The former were asked to be both pedagogical and engaging in their talks, presenting their techniques in terms comprehensible to theoretical physicists, but also stimulating discussion and interactions by pointing out the frontiers and grey areas in experimental understanding.

The central location in Turin was a very efficient and agreeable venue, providing excellent facilities, transport, and restaurant and hotel services at reasonable prices.

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. Important advances were made in structuring both the ETSF and the different themed collaboration teams, many of which echo specific preoccupations of Psi-k: electron correlation, electron-vibration coupling, and the simulation of large and/or biological systems. Several of the teams will submit workshop proposals to Psi-k in the coming application periods, as a result of organization carried out during this meeting.

Main themes addressed

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 challeng-

ing experimentally, and were presented by Julia Stähler (FHI Berlin) and Franck Lépine (CNRS U Lyon), 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 invited speakers Fausto Rossi (Politecnico Torino) and Alexander V. Soudackov (Penn State), covering both advanced open quantum systems and non-adiabatic time evolution - two crucial topics linking time resolved and transport spectroscopies (see next subsection).

Nanoscale electron transport The transport properties of nano and atomic scale systems are the future of electronic devices, and one of the main driving forces for applied research in materials science. Latha Venkataraman (Columbia University) presented her ground breaking work on making nanoscale junctions reproducible, functional, and on understanding the electronic states and dynamics which determines the final macroscopic observables. Her existing collaborations with theoreticians in Density Functional Theory provided a clear demonstration of the symbiosis this conference wished to foster. The complex many-body physics which has been revealed in certain partly filled and spin-dependent nanoscopic junctions was Erio Tosatti (ICTP Trieste)

Photoemission spectroscopy The delicate nanoscale manipulation of electronic properties was demonstrated by Alexander Grüneis (U Vienna) who has tuned the band gap and electron phonon coupling of graphene through functionalization under CVD. Using angle resolved photoemission experiments exquisitely detailed information on electronic bands can be obtained, and compared directly to theoretical calculations, in particular many-body perturbation theory (MBPT). Two powerful and new implementations of MBPT were presented by Xavier Blase (CNRS Grenoble) using a Gaussian basis set for very large systems and by Stefan Blügel (FZ Jülich) using the FLAPW formalism for all-electron precision and heavy-element systems.

Vibrational spectroscopies Vibrational spectroscopies have several intersections with the themes mentioned above, through adiabatic effects and low energy excitations or renormalizations, and also stand alone as very popular and powerful tools for molecular and materials analysis. Johannes Neugebauer (U Braunschweig) presented systematic chemical-accuracy calculations of vibrational structure in large systems and resonant Raman spectroscopy. Nedjma Bendiab (U Lyon) studies nanoscale carbon structures using Raman and local probe microscopies. Long standing mysteries about the vibrational modes of graphite, graphene and carbon nanotubes can be answered and explained microscopically using these techniques.

Conclusion

The ETSF 2011 conference was a very successful edition, both through the rich interactions and the high quality of the experimental 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, MaiMoSine, 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 Coimbra in Portugal, and return to the core business of the ETSF in the development of theory, algorithms, and code for the calculation of electronic excited states, and the wide variety of electronic correlations.

Program

Tuesday 27 September
Opening
Ultrafast changes of lattice symmetry at the onset of the photoinduced insulator-metal transition of VO2, Julia Staehler
Microscopic theory of energy dissipation and decoherence in open quantum devices, Fausto Rossi
Theoretical studies of ultrafast photoinduced proton-coupled electron transfer reactions, A.V. Soudackov
Coffee Break
Non-linear phenomena in time-dependent density-functional theory: What Rabi physics can teach us, Johanna Fuks
Size-consistency and fractional spin in Reduced Density-Matrix Functional Theory, Nicole Helbig
Exact exchange-correlation potentials for steady-state and time-dependent electronic systems, James Ramsden
Lunch
First-principles GW and BSE calculations for molecules of interest for organic photovoltaic applications, Xavier Blase
Physics with short light pulses: experiments and perspectives, Franck Lépine
First-principles study of the electronic and optical properties of ZnO and ZnS wurtzite nanoclusters, Giuliano Malloci
Exploring the conformations, stability, and dynamics of helix-forming alanine-based polypeptides: first-principles predictions and benchmarks, Mariana Rossi
Ab initio electronic spectra of peptides, Elena Molteni Effects of N-doping on the electronic properties of carbon atomic chains with distinct sp2 graphene-like terminations, G. Gueorguiev
Welcome Aperitif
ETSF general meeting CT reports and meetings

Wednesday 28 September
Electronic properties of functionalized graphene Alexander Gruneis
The GW approximation in the FLAPW method: Applications to Oxides and Topological Insulators, Stefan Blügel
Satellites in Valence Photoemission Spectroscopy, Matteo Guzzo
Coffee Break
Exotic quasi-one-dimensional systems: graphene-based superlattices, Lars Matthes

Optical response calculations of gold alloys from first principles, Deniz Kecik
Strong excitons in novel two-dimensional crystals: graphane, silicane and germanane, Friedhelm Bechstedt
Lunch + Poster Session
Towards a novel approach for the calculation of many-body Green's functions, Giovanna Lani
Exact solution for 2-particle Green's function: an alternative to Bethe Salpeter Equation, Lorenzo Sponza
Strong electronic correlation in the Hydrogen chain: a variational Monte Carlo study, Lorenzo Stella
Properties of the screened interaction in finite systems, Adrian Stan
Coffee Break
GW/BSE Calculations of X-ray Spectra, John Vinson
Many-pole models of inelastic losses and satellites in x-ray spectra, Joshua Kas
Solids under intense ultrafast excitations: a time-dependent Bethe-Salpeter approach, Andrea Marini
ASE: A programmable environment for calculations with many electronic structure codes, Ask Hjorth Larsen
The PRACE infrastructure Micael Oliveira
Short GUI demos, Massimo Conter, Flavio Abreu Araujo

Thursday 29 September
Kondo screening and antiscreening in electron transport across metallic and molecular magnetic nanocontacts, Erio Tosatti
Electronics and Mechanics of Single Molecule Circuits, L. Venkataram
Spatio-Temporal description of Quantum Transport, Björn Oetzel
Coffee Break
Ab initio many-body effects in TiSe2, Marco Cazzaniga
Electronic Structure of Dye-Sensitized TiO2 Clusters from G0W0, Noa Marom
Multi-pole models for the approximation of spectral properties in GW, Martin Stankovski
Lunch + Poster Session
Probing Excited-State Potential-Energy Surfaces by Theoretical Resonance Raman Spectroscopy, J. Neugebauer
Electronic and mechanical properties of sp carbon atomic nanowires, Nicola Manini
Electron-phonon coupling in STO, Bin Xu
Coffee Break
Bootstrap approximation for the exchange-correlation kernel of time-dependent density functional theory, S. Sharma
Special Quasirandom Structures: application to liquid systems, A. Mosca Conte
A unified description of ground and excited state properties of finite systems: the self-consistent GW approach, Fabio Caruso
Simple preconditioning for time-dependent density-functional perturbation theory, L. Lehtovaara
Social Dinner

Friday 30 September
Unravelling the properties of graphene and nanotubes with Raman spectroscopy, N. Bendiab
NMR and EPR with Density Functional Perturbation Theory, S. de Gironcoli
Coffee Break
The polarizability and hyperpolarizability of C and BN nanotubes. A quantum-mechanical simu- lation, Roberto Dovesi
Auger Recombination and Impact Ionization from first-principles: from bulk to nanocrystals, Marco Govoni
Excited state properties of TiO2 surfaces and nanostructures, Letizia Chiodo
Optical characterization of Au nanowires on Si(111) surfaces, Conor Hogan
Lunch
Phase transitions within the GW approximation, Matteo Gatti
Momentum Distribution and Renormalization Factor in Sodium and the Electron Gas, Valerio Olevano
Current issues in the description of charged defects: the case of hydrogen in amorphous silica, David Waroquiers
Coffee Break
Insights in the T-matrix approximation, Pina Romaniello
TDDFT dynamics for strongly correlated model systems, Claudio Verdozzi
Closing remarks
Collaboration Teams Meetings

Participant list

Adrian Stan, University of Jyvaskyla
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