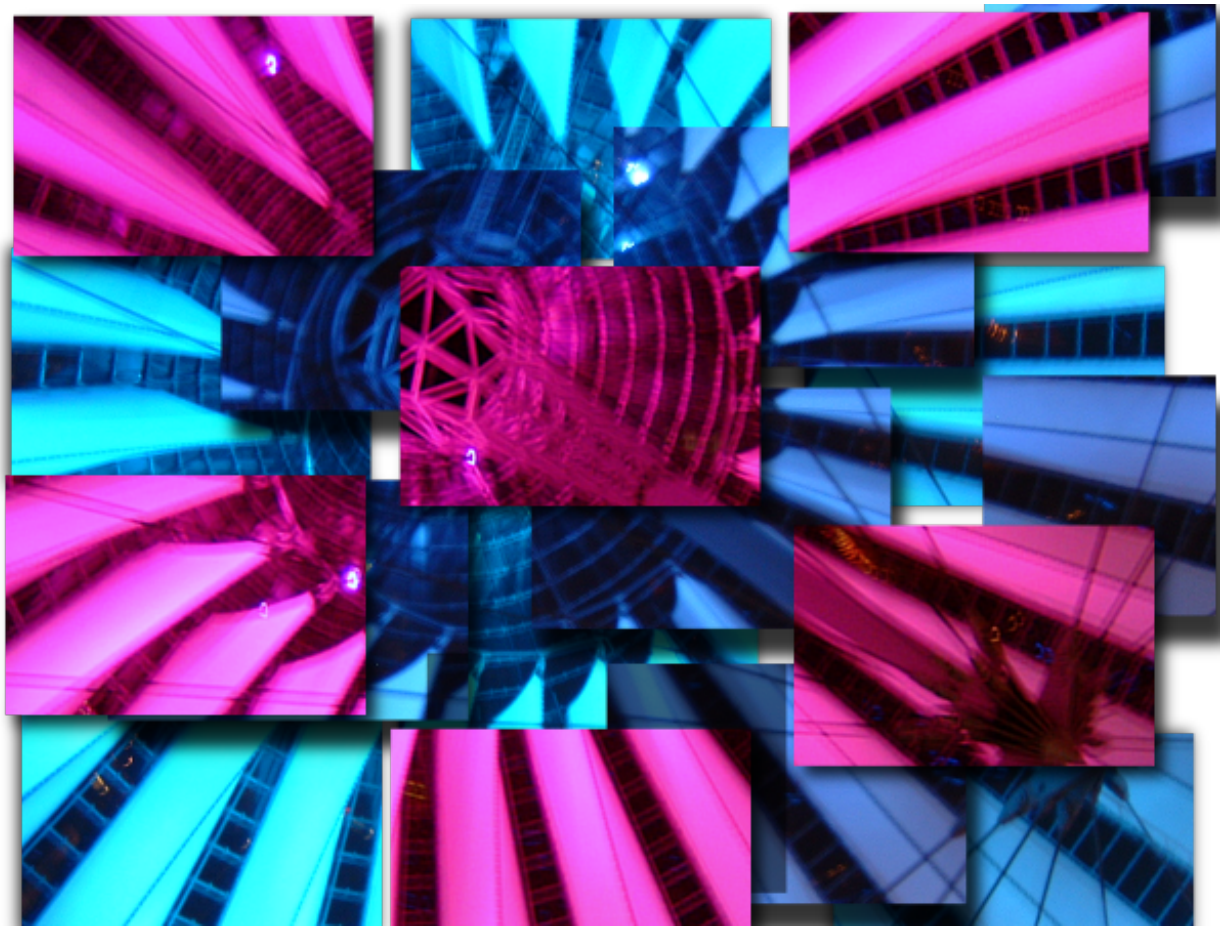
15th ETSF Workshop on Electronic Excitations

New Frontiers in Theoretical Spectroscopy and Quantum Transport



Berlin, 12-15 October 2010

Nanoquanta-ETSF series of workshops

- **New Frontiers in Theoretical Spectroscopy and Quantum Transport**

  15th Nanoquanta-ETSF Series of Workshops on Electronic Excitations

  Berlin (Germany) [11-15 October 2010]

- **Ab-initio tools for the characterization of nanostructures**

  14th in the Nanoquanta-ETSF Series of Workshops on Electronic Excitations

  Evora (Portugal) [14-19 September 2009]

- **Theoretical Spectroscopy and Quantum Transport**

  13th in the Nanoquanta-ETSF Series of Workshops on Electronic Excitations

  Pugnochiuso-Vieste (Italy) [22-27 September 2008]

- **Time Dependent Density Functional Theory: Advances and Prospects**

  12th in the Nanoquanta-ETSF series of Workshops

  Aussois (France) [18-22 September 2007]

- **A decade of applications of the Bethe-Salpeter Equation**

  11th in the Nanoquanta-ETSF series of Workshops

  Houffalize (Belgium) [19-22 September 2006]

- **40 Years of the GW Approximation for the Electronic Self-Energy**

  10th in the Nanoquanta-ETSF series of Workshops

  Bad Honnef (Germany) [12-15 September 2005].

- **Theory and Modeling of Electronic Excitations in Nanoscience**

  9th in the Nanoquanta-ETSF series of Workshops

  Maratea (Italy) [19-23 September 2004]

- **Ab initio Electrons Excitations Theory: Towards Systems of Biological Interest**

  8th in the Nanoquanta-ETSF series of Workshops

  San Sebastián (Spain) [21-24 September 2003]

- **Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials**

  7th in the Nanoquanta-ETSF series of Workshops

  Lyon (France) [23-25 September 2002]

- **Excited states and electronic spectra**

  6th in the Nanoquanta-ETSF series of Workshops

  Lyon (France) [20-22 July 2000]

- **Calculation of Electronic Excitations in Finite and Infinite Systems**

  5th in the Nanoquanta-ETSF series of Workshops

  Lyon (France) [1-3 September 1999]

- **Spectroscopy of Electronic Excitations in Materials**

  4th in the Nanoquanta-ETSF series of Workshops

  Valladolid (Spain) [7-9 September 1998]

- **Electronic Exchange and Correlation in Advanced Materials**

  3rd in the Nanoquanta-ETSF series of Workshops

  Lyon (France) [11-12 September 1997]

- **Electronic Exchange and Correlation in Advanced Materials**

  2nd in the Nanoquanta-ETSF series of Workshops

  Palaiseau (France) [26-28 September 1996]

- **Electronic Exchange and Correlation in Advanced Materials**

  1st in the Nanoquanta-ETSF series of Workshops

  Rome (Italy) [September 1995]

15th ETSF Workshop on Electronic Excitations:
New Frontiers in Theoretical Spectroscopy and Quantum Transport
Berlin (Germany), 12-15 October 2010

Scientific Report

The workshop gathered 112 participants from leading international groups. There were 39 oral presentations (18 invited speakers and 21 contributed talks) and 34 posters. The workshop allowed the participants to discuss the advances in the theoretical and computational treatment of optical and dielectric spectroscopy as well as quantum transport in the framework of many-body-perturbation-theory (MBPT).

Invited speakers from leading international groups gave an in-depth overview of current research activities in MBPT (and related fields) and placed recent results into context. Young researchers (Ph.D. students and post-docs) also had the opportunity to present their work (more than half of the oral presentations were given by non-permanent researchers).

The workshop started with a short session (2 speakers) devoted to some recent developments in DFT and their application. It was followed by a longer session (4 speakers) devoted to trying to go beyond the electronic picture. Some recent experimental advances in the field were first presented. Then, three different theoretical approaches were discussed. The first day ended with a session devoted to methodological developments (4 speakers) going from faster approaches to perform the calculations to better accuracy in describing the van de Waals interaction.

The second day was devoted to presenting new theoretical developments. Density matrix functionals and local correlation methods were first presented. An alternative to the self-energy was also proposed by direct calculation of the one particle Green's function. Then, an interesting bridge between quantum electrondynamics (QED) and MBPT was discussed. A talk was devoted to improving the self-consistency in the GW approximation. Another presented an approach to get rid of self-interaction in exchange and correlation functionals using ensemble-DFT. The last talk proposed some developments to take magnetic fields into account.

The third day started with a session on bio-molecules (3 speakers). After a talk devoted to recent experimental advances in this topic, two talks presented some results obtained using theoretical spectroscopy to study peptides. The second session (5 speakers) focused on quantum transport whose importance has increased in the MBPT community. Indeed, the Green's functions formalism at the heart of MBPT is also particularly well suited to describe electronic quantum transport. Currently, it is used both in the Landauer-Büttiker approach and

in the non-equilibrium Green's functions (NEGF) theory, also known as Keldysh formalism. During the session, there were a lot of discussions about whether or not DFT can predict the conductance accurately, and if including correlations at the MBPT level can be a solution when DFT fails. Approaches based on TDDFT have also been presented in this session. Finally, a session (3 speakers) was devoted to some recent applications of MBPT including magnetic insulators, excitons in zinc oxyde, and spin excitations in magnetic multi-layers.

The last day started with a session (4 speakers) about TDDFT applications going from nanocrystals to interesting crystalline structures passing through the modification of the optical properties of paper due to ageing. The second session (2 speakers), presenting some applications of MBDT, was in fact the end of the last session of the third day. The two talks focused on oxides. The next session (3 speakers) was devoted to carbon nanostructures. One of the talk presented an interesting building-block approach, while the other two focused on graphane and fuorinated graphene respectively. The last session (2 speakers) of the workshop was devoted to properties going beyond linear regime. It included a talk on recent experimental advances in the field.

Besides the oral presentations, a poster session was also organized. It gave rise to very interesting discussions. Indeed, wide variety of subjects were being presented and the discussions went well beyond these subjects. The meeting provided an informal atmosphere for stimulating discussions between researchers working in this exciting field. New collaborations were initiated following these discussions.

This workshop has been a real success. On the one hand, it helped increasing the collaborations (in order to develop theory and codes) between the various actors of the field. On the other hand, it contributed to the development and the spread of the know-how.

Hereafter, we have attached the conference program.

Programme

Monday 11	
09:00	ETSF Steering Committee
17:00	Registration
	ETSF Steering Committee
20:00	Dinner

Tuesday 12	
09:00	Welcome
09:30	Bersier
10:00	Odashima
10:20	Coffee Break
10:50	Wolf
11:20	Cannuccia
12:00	Lunch
14:30	Biermann
15:00	Karlsson
15:30	Coffee Break
16:00	Furche
16:30	Foerster
16:50	Berger
17:10	Tkatchenko
17:30	Poster Up
18:30	Dinner
20:00	Poster Session

Wednesday 13	
09:00	Pernal
09:30	Schütz
10:00	Lani
10:20	Coffee Break
10:50	Olevano
11:10	Kresse
11:30	Gidopoulos
11:50	Marini
12:10	Lunch
14:30	General Meeting
15:00	CT Grand Challenges
16:00	Coffee Break
16:30	Software Meeting
18:30	Dinner
20:30	Advisory Board

Thursday 14	
09:00	Weightman
09:30	Molteni
10:00	Blum
10:30	Coffee Break
11:00	Dash
11:30	Mera
11:50	Myöhänen
12:10	Lunch
14:30	Rangel
15:00	García-Lastra
15:30	Coffee Break
16:00	Rödl
16:30	Schleife
16:50	Sasioglu
17:10	CT Grand Challenges
20:00	Social Dinner

Friday 15	
09:00	Guerra
09:20	Mosca Conte
09:40	Colombo
10:10	Sponza
10:30	Coffee Break
11:00	Guzzo
11:20	Iacomino
12:10	Lunch
14:30	Hambach
15:00	Cudazzo
15:20	Sahin
15:40	Coffee Break
16:10	Bertocchi
16:30	Sipe
17:00	Closing Remarks
19:00	Dinner

Saturday 16	
09:00	ETSF Steering Committee
10:30	Coffee Break
11:00	ETSF Steering Committee
12:30	Lunch
Departures	

Monday 11 October

17:00-20:00 Registration

Tuesday 12 October

09:00 Welcome

9:30-10:20 DFT Development and Application

09:30 Christophe Bersier (*Max-Planck Institute for Microstructure Physics, Halle*)
Density functional theory at finite temperature: Towards an ab-initio description of phase transitions

10:00 Mariana Odashima (*Max-Planck Institute for Microstructure Physics, Halle*)
Improving the Lieb-Oxford condition in PBE for atoms, molecules and solids

10:20-10:50 Coffe Break

10:50-12:00 Beyond the electronic picture (I)

10:50 Martin Wolf (*Fritz-Haber-Institut, Berlin*)
Ultrafast dynamics of complex materials analyzed with time-resolved photoelectron spectroscopy

11:20 Elena Cannuccia (*University of Rome "Tor Vergata"*)
Giant polaronic effects in polymers: breakdown of the electronic picture

12:00-14:30 Lunch

14:30-15:30 Beyond the electronic picture (II)

14:30 Silke Biermann (*CPHT, Ecole Polytechnique, Palaiseau*)
Electronic Structure of Correlated Materials from First Principles – a Dynamical Mean Field Point of View.

15:00 Daniel Karlsson (*Lund University*)
A TDDFT + DMFT approach to the real-time dynamics of 3D strongly correlated model systems.

15:30-16:00 Coffe Break

16:00-17:30 Methods Developments

16:00 Filipp Furche (*University of California, Irvine*)
Fast Computation of Molecular RPA Correlation Energies by Resolution-of-the-Identity and Imaginary Frequency Integration

16:30 Dietrich Foerster (*Université de Bordeaux*)
Improved calculational methods for organic semiconductors

16:50 Arjan Berger (*Ecole Polytechnique, Palaiseau*)
Ab initio calculations of electronic excitations: Collapsing spectral sums

17:10 Alexandre Tkatchenko (*Fritz-Haber-Institut der MPG, Berlin*)
Towards accurate van der Waals interactions in complex materials

17:30-18:30 Poster Up

18:30 Dinner

20:00 Poster Session

Wednesday 13 October

09:00-10:20 Theory Developments (I)

09:00 Katarzyna Pernal (*Technical University of Lodz*)
Response and excitation energies from Density Matrix Functionals

09:30 Martin Schütz (*University of Regensburg*)
Local correlation methods for excited state calculations of extended systems

10:00 Giovanna Lani (*Ecole Polytechnique, Palaiseu*)
Direct calculation of the one particle Green's function: an alternative to the self-energy

10:20-10:50 Coffe Break

10:50-11:50 Theory Developments (II)

10:50 Valerio Olevano (*Institut Neel, Grenoble*)
Many-body theory in relativistic covariant form: bridging QED to MBPT

11:10 Georg Kresse (*University of Vienna*)
Selfconsistent GW via the selfconsistent solution of the Sham-Schlüter equation

11:30 Nikitas Gidopoulos (*Rutherford Appleton Laboratory, Didcot*)
Ghost-self-interaction-free exchange and correlation functionals for the ensemble-density-functional theory for excited states

11:50 Andrea Marini (*University of Rome "Tor Vergata"*)
Carbon nanotubes in confined magnetic fields: Aharonov-Bohm oscillations and persistent currents from a new perspective

12:10-14:30 Lunch

14:30-15:00 General Meeting

15:00-16:00 Collaboration Teams Grand Challenges

16:00-16:30 Coffe Break

16:30-18:30 Software Meeting

18:30-20:30 Dinner

20:30 Advisory Board Meeting

Thursday 14 October

09:00-10:30 Bio-molecules

09:00 Peter Weightman (*University of Liverpool*)
Probing the structure and dynamics of biomolecules adsorbed on surfaces.

09:30 Elena Molteni (*University of Milan*)
Electronic spectra of peptides: effects of conformational changes

10:00 Volker Blum (*University of California, Irvine*)
Structure, spectroscopy and dynamics of peptides in the gas phase

10:30-11:00 Coffe Break

11:00-12:10 Quantum Transport (I)

11:00 Louise Dash (*University of York*)
Can the Landauer formula for the current be used for non-equilibrium steady-state interacting systems?

11:30 Hector Mera (*CEA, Institute for Nanoscience and Cryogenics, Grenoble*)
Are DFT conductances accurate?

11:50 Petri Myöhänen (*University of Jyväskylä*)
Kadanoff-Baym approach to time-dependent quantum transport in AC and DC fields

12:10-14:30 Lunch

14:30-15:30 Quantum Transport (II)

14:30 Tonatiuh Rangel (*Université catholique de Louvain-la-Neuve*)
Transport properties of molecular junctions from Many-Body Perturbation Theory

15:00 Juan María García-Lastra (*Universidad del País Vasco, San Sebastián*)
Computational Design of Chemical Nanosensors: Metal Doped Carbon Nanotubes

15:30-16:00 Coffe Break

16:00-16:50 MBPT Applications (I)

16:00 Claudia Rödl (*Friedrich-Schiller-Universität, Jena*)
Optical Properties of Magnetic Insulators: Absorption Spectra and Bound Excitonic States

16:30 André Schleife (*Friedrich-Schiller-Universität, Jena,*)
Heavy n-doping: Wannier-Mott and Mahan excitons in ZnO

16:50 Ersoy Sasioglu (*Forschungszentrum Jülich*)
Effective Coulomb interaction and spin excitations in $L1_0$-type magnetic multilayers from many-body perturbation theory

17:10-19:30 Collaboration Teams Grand Challenges

20:00 Social Dinner

Friday 15 October

09:00-10:40 TDDFT Applications

09:00 Roberto Guerra (*Università di Modena e Reggio Emilia*)
Local-Field Effects in Si/SiO_2 Nanocrystals

09:20 Adriano Mosca Conte (*Università di Roma Tor Vergata*)
Theoretical investigation on paper optical properties modifications induced by ageing

09:40 Luciano Colombo (*Università di Cagliari*)
Quantum confinement in nanocrystalline silicon

10:10 Lorenzo Sponza (*Ecole Polytechnique, Palaiseu*)
Calculated optical spectrum of $SrTiO_3$ cubic structure

10:30-11:00 Coffe Break

11:00-11:40 MBPT Applications (II)

11:00 Matteo Guzzo (*Ecole Polytechnique, Palaiseau*)
Exchange an Correlation effects in the electronic properties of semiconductors and transition metal oxides

11:20 Amilcare Iacomino (*Universidad del País Vasco, San Sebastián*)
Unraveling the optical properties of TiO_2 nanostructures from ab-initio Many-Body techniques

12:00-14:30 Lunch

14:30-15:40 Carbon Nanostructures

14:30 Ralf Hambach (*Ecole Polytechnique, Palaiseau*)
Electron Energy-Loss in Carbon Nanostructures: a Building-Block Approach

15:00 Pierluigi Cudazzo(*Universidad del País Vasco, San Sebastián*)
Strong Charge-Transfer Excitonic Effects and the Bose-Einstein Exciton Condensate in Graphane

15:20 Hasan Sahin (*Bilkent University*)
Half and Fully Fluorinated Graphene

15:40-16:10 Coffe Break

16:10-17:00 Beyond Linear Regime

16:10 Matteo Bertocchi (*Ecole Polytechnique, Palaiseau*)
The optical properties if Si/CaF2 multi-quantum wells: role of size and interface configuration

16:30 John Sipe (*University of Toronto*)
Non-linear optics and coherent injection

17:00 Closing Remarks

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