Research Networking Programmes

Science Meeting – Scientific Report

The scientific report (WORD or PDF file - maximum of seven A4 pages) should be submitted online within two months of the event. It will be published on the ESF website.

***Proposal Title**: ETSF Young Researchers' Meeting 2014: evolution of ab-initio methods for condensed matter - connection with experiments and industry*

Application Reference N°: 5242

1) Summary (up to one page)

The European Theoretical Spectroscopy Facility (ETSF) (formerly NANOQUANTA) is a network of more than 200 researchers from Europe and U.S.A., who develop state-of-the-art theoretical and computational methods in condensed matter physics. The network facilitates the collaboration and the rapid transfer of knowledge between researchers, and its main objective is to provide knowledge and expertise in the field of theoretical spectroscopy, to broaden the access of the public and private sector to these tools.
Starting in 2004, the young researchers within the ETSF have organized, in different European countries, an annual Young Researchers' Meeting (YRM). Organized and attended only by Ph.D. students and postdocs, it offers them the chance to start new collaborations, to exchange ideas, techniques and know-how, and to improve their presentation, communication and organizational skills.
Organized in Rome, the YRM-2014 had 60participants, including 3 researchers from 3 companies across Europe. Their participation, and the presence of a special Experiment-Industry Day, was aimed at encouraging future collaborations and initiative, and at involving theoreticians in projects of industrial interest. Aside from presenting their work, the speakers have been asked to highlight the key components, of their respective research lines, that could greatly benefit from an interaction with theoreticians.

2) Description of the scientific content of and discussions at the event (up to four pages)

The 5 days conference was divided in 6 sections and one Experiment-Industry Day – as mentioned in Section 1. The goal was to offer a comprehensive and detailed overview of the research carried out within the ETSF network, and to maximize the opportunity for newcomers to present their work. The 6 sections were:

- Ground state properties
- Photoemission
- Optical properties
- Electron-phonon interaction
- Quantum transport
- New theoretical methods

GROUND STATE PROPERTIES

The ground state is the lowest energy state of a quantum mechanical system. While most real-life processes deal with excited states, the ground state properties of a system constitute the starting-point for condensed-matter calculations. For this reason, accurate knowledge of the ground state is of paramount importance in the field.

The Density Functional Theory (DFT) has recorded a sounding success in reproducing and predicting the ground state properties of surfaces, bulk crystals and molecules. In most cases the comparison with experiments is excellent: structural details of a wide variety of solids and molecules are predicted within an error of 1% compared to the experiments. Many other properties such as vibrational spectrum, bulk modulus and dielectric constants can be accurately calculated. In recent years, Quantum Monte Carlo (QMC) methods emerged as a reliable and alternative theoretical approach to tackle problems of chemical interest and include electronic correlations.

Mainly focused on organic systems, but also on semiconductors, the section has brought forward the need for temperature-dependent formalisms meant to study phenomena at room temperature. The application of QMC to biological systems – presented in the talk of E. Coccia - revealed differences in the calculation of the bond alternation of polyenic chains with respect to the DFT calculations. If the molecular vibrations are harmonic this gives a correct evaluation of this compounds even at room temperature and consequently a better estimation of the optical properties of important biological molecules such as rhodopsin.

PHOTOEMISSION

Theoretical spectroscopy is concerned with simulating the interaction between matter and radiated energy. The main purpose of theoretical spectroscopy is to facilitate the interpretation of experiments through modelling the phenomena that result from this interaction. As many experimental techniques deal with charged electronic excitations, i.e., photoemission spectroscopy or inverse photoemission spectroscopy, in general, DFT is not appropriate to describe these excitations. One of the most suitable approaches to study excited state properties of semiconductors, insulators and molecular systems is the Many Body Perturbation Theory (MBPT) based on Green functions. Within this framework, the GW approximation for the self-energy is the most widely used and reliable.

Falk Tandetzky opened the section on photoemission. His talk discussed a general approach to the GW approximation, the existence of multiple solutions, and gave an overview on the use of this method. The section further touched on the problem of applying the GW approximation to transition metal oxides (a hot topic in energy-related applications) and on going beyond GW, into the strongly correlated regime, by developing new, GW-based methods.

OPTICAL PROPERTIES

Neutral electronic excitations are strictly related to optical properties – photoluminescence, absorption and Raman spectroscopy. These are among the most difficult properties to describe by ab-initio methods because of the need to evaluate the contribution of the electron-electron and electron-hole interaction to the optical spectrum.

In condensed matter the methods of choice for calculating optical properties are based on the solution of the Bethe-Salpeter equation, or on Time Dependent Density Functional Theory (TDDFT). Both formalisms are in principle exact, but their application in a real many-electron interacting system requires several approximations. The suitability in using one or the other theory depends on the geometrical and chemical properties of the system, and on the kind of information that one would like to extract from these calculations. The computational cost considerably reduces the number of possible applications – the existent studies currently deal with very small systems.

Our invited speaker Daniele Varsano, and international expert on these matters, gave a review talk on the subject in which he showed results on neutral excitations in a large variety of systems ranging from condensed matter to biological physics. The section furthered the application of MBPT and TDDFT to challenging systems and underlined the need for a time-dependent regime.

ELECTRON-PHONON INTERACTION

The electron-phonon coupling is responsible for many phenomena, from superconductivity and termal-transport, to piezoelectricity. Most of the theoretical studies of these physical processes are based on phenomenological approaches that have been used with great success to describe existing experiments. However, prediction and design of new materials still remains a great challenge. This is the reason why ab-initio calculations could induce a great improvement.

A very important step in this direction has been done by M. Cardona and more recently by E. Cannuccia and A. Marini, who – using ab-initio calculations – demonstrated the importance of the electron-phonon coupling in spectroscopy. In particular, E. Cannuccia and A. Marini proved that, besides its importance in metals and in materials at finite temperature, the electron-phonon coupling covers a very important role also in insulators at very low temperature. They showed that the quantum zero-point motion of the carbon atoms induces strong effects on the optical and electronic properties of diamond and trans-polyacetylene. E. Cannuccia was the invited speaker for this section. During the latter, the importance of electron-phonon interaction in organic systems was highlighted as well as the underestimation of electron-phonon coupling in DFT-LDA calculations.

QUANTUM TRANSPORT

Power consumption, heat dissipation and quantum effects constitute the three major limitations on the road to miniaturization of electronic devices. At nanoscale level, new materials have

been suggested in order to circumvent the limits of conventional technology. It is then crucial to have an accurate description – both qualitatively and quantitatively – of electronic transport through such nanoscale devices.

The most popular methods for electronic transport are based on the Kubo and the Landauer-Buttiker formalisms. However, in the last decade, DFT has become the standard method also in this field. Albeit successful in the qualitative description, DFT has proven to be inadequate for many systems since electronic correlations can have a big impact in the description of currents and electronic densities. Therefore, as strongly correlated systems are out of reach for DFT calculations, the method of choice becomes the MBPT. However limited by the computational cost, the development of novel ab-initio techniques based on the GW method have been applied with success to molecules, junctions, graphene and several other systems.

The invited speaker of this session has been Elham Khosravi, an international expert in time-dependent phenomena in quantum transport. Her talk gave a comprehensive overview of the progress in the field and pushed in the direction of temperature dependent phenomena. As in the section dedicated to Ground State Properties, also here we have seen the importance of formalisms capable of providing accurate descriptions of physical phenomena over a wide range of temperatures. The discussion continued in the section with the case of magnetic transport and application of time-dependent formalisms to large, graphene flakes, emphasizing the role of bond alternation and edge-effects in the description of current.

THEORETICAL DEVELOPMENTS

The discovery of new materials and innovation of experimental techniques prompts the development of new theoretical methods in the field of condensed matter physics. Because of the extremely wide range where these developments occur, this section didn't have an introductory talk. More than in other sections, the discussions were driven by the subject of the talks, ranging from harmonic generation and DFT to applications of mathematical concepts in physics.

It has emerged that the forefront of new theoretical methods development, within ETSF, currently includes surface physics, correlated dynamics and concepts from mathematical physics applied to condensed matter. All these efforts aim to a better description of emergent phenomena at nano- and molecular-scale.

3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

The event brought together 53 young researchers and 3 companies from 10 countries. Not only it fostered the connections between academia and industry, but also helped covering the gap between experimental and theoretical research.
For the ETSF network, this was the 11th YRM event, and a step forward in its consolidation .
The feedback within the network was extremely positive, and we concluded that this series of events will continue in 2015 with the Young Researchers' Meeting in Paris, organized by the ETSF node in Palaiseau, University of Sorbonne and College de France.

The goal of this conference was to bring together young researchers and give them the opportunity to share their results in a friendly environment, to practice their presentation skills and allow them start new collaborations. At the same time, the Experiment-Industry Day was designed to enrich the perspective of young researchers and to drive an interaction between

theoretical developments and industry, through developing or applying the theoretical methods to experimental data.

In the context of ab-initio calculations, during the workshop it became clear that the development of formalisms with the capability to study physical phenomena at room temperature is a priority. In this respect, evaluating the state of degradation of precious artefacts is a prime example of the fundamental importance of the joint effort between developing such methods and emerging experimental techniques. Another example is the prediction of current through molecular junctions at room temperature.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

Day 1 - May, 12th 2014
Experimental-industrial

- 09:00 to 09:30 - Registration
- 09:30 to 10:00 - Welcome
- 10:00 to 10:40 - **Adriano Violante**
  Indirect Exciton Transport and Manipulation by Confined Acoustic Potentials
- 10:40 to 11:20 - **Eugen Speiser**
  Investigation of Reconstructed Surfaces by Optical and Vibrational Properties
- 11:20 to 11:40 - Coffee Break
- 11:40 to 12:20 - **Stefano Schutzmann**
  Spectroscopic Ellipsometry for the Characterization of Nanostructured Thin Films: State-of-the-art and Future Perspectives
- 12:20 to 14:00 - Lunch
- 14:00 to 14:40 - **Linda Riele**
  Analysis of Various Components of Body Fluids Applying Photometry
- 14:40 to 15:20 - **Benjamin Buick**
  In-situ Metrology for Advanced Process Control
- 15:20 to 15:45 - **Lorenzo Teodonio**
  Why is the Leonardo da Vinci Self-Portrait Yellowed ?

poster session

- 15:45 to 18:00 - Poster Session

Day 2 - May, 13th 2014

Photoemission

- 09:00 to 09:50 - **Falk Tandetzky**
  Symmetry Breaking, Hartree Fock, GW and Extra Solutions
- 09:50 to 10:15 - **Matteo Gerosa**
  Computing the Electronic Properties of Wide Band Gap Oxides for Energy Applications: Hybrid Functional and GW Calculations
- 10:15 to 10:40 - **Sophie Chauvin**
  How to Map Non-Local Interactions onto Dynamical ones: the Hubbard Dimmer
- 10:40 to 11:00 - Coffee Break
- 11:00 to 11:40 - **Matteo Guzzo**
  Satellite structures in photoelectron spectroscopy: What, Where and Why?

Ground state

- 11:40 to 12:05 - **Efterpi Kalesaki**
  Quantum Confinement and Strain Induced Modifications in the Lattice Dynamics of PbSe
- 12:05 to 12:30 - **Andreas Stegmueller**

Precursor Chemistry, Growth Characteristics and Interface Phenomena of Gallium Phosphide Epitaxially Grown on Si(001): Elucidating Elementary Processes by DFT

- 12:30 to 12:55 - **Simon M.-M. Dubois**
  Preconditioning and Parallel Propagation of Support Functions for Total-Energy Calculation within the Optimal Basis Density-Matrix Minimization Approach.
- 12:55 to 14:35 - Lunch
- 14:35 to 15:00 - **Henrique Pereira Coutada Miranda**
  Vibrational Properties of Graphene on a Substrate
- 15:00 to 15:25 - **Nathaniel Raimbault**
  Magnetization in Extended Systems Within Time-Dependent Current-Density-Functional Theory (TDCDFT)
- 15:25 to 15:50 - **Yael Bronstein**
  Quantum-Driven Phase Transition in High-Pressure Ice
- 15:50 to 16:10 - Coffee Break

Electron-phonon

- 16:10 to 16:50 - **Elena Cannuccia**
  Finite Temperature Calculations of the Electronic and Optical Properties of Solids and Nanostructures
- 16:50 to 17:15 - **Carina Faber**
  GW Many-Body Perturbation Theory for Electron-Phonon Coupling Calculations
- 17:15 to 17:40 - **Tamas Demjan**
  Near-degenerate Quasi-particle States and Level Crossings Induced by Electron-vibration Self-interaction.

Day 3 - May, 14th 2014

New methods

- 09:00 to 09:25 - **Jonathan Laflamme Janssen**
  Faster G0W0 Implementation for More Accurate Material Design
- 09:25 to 09:50 - **Stefano Di Sabatino**
  RDMFT ↔ MBPT: mutual insight into electron correlation
- 09:50 to 10:15 - **Valerio Rizzi**
  Correlation: the Key to Energy Feedback in Radiation Damage
- 10:15 to 10:40 - **Jianqiang Zhou**
  Improved Description of Electron-Plasmon Coupling in Green's Function Calculations
- 10:40 to 11:00 - Coffee Break
- 11:00 to 11:25 - **Wael Chibani**
  Self-consistent Dynamical Embedding In Real Space
- 11:25 to 11:50 - **Nicolas Tancogne-Dejean**
  Real Space investigation of local field effects on surfaces
- 11:50 to 12:15 - **Adrian Stan**
  On the Problem of Excitations and Energy Transfer in MBPT

Quantum transport

- 12:15 to 13:05 - **Elham Khosravi**
  Time-Dependent Phenomena in Quantum Transport

- 13:05 to 14:45 - Lunch
- 14:45 to 15:10 - **Adela Nicolaev**
  Transport in Ferrocene Single Molecules with Spinning Rings
- 15:10 to 15:35 - **Marco Di Gennaro**
  Ab-initio Calculations of Spin Dependent Seebeck Effect in Permalloy
- 15:35 to 15:55 - Coffee Break
- 15:55 to 16:20 - **Riku Tuovinen**
  Quantum Dynamics in Graphene Nanoribbons
- 16:20 to 16:45 - **Micaela Matta**
  Simulations of Complex Materials: the First Liquid Crystal Based on a Trimetallic Nitride Template Endohedral Metallofullerene (TMT-EMF)

Day 4 - May, 15th 2014

Optical properties

- 09:00 to 09:50 - **Daniele Varsano**
  TDDFT and MBPT for the calculation of optical properties
- 09:50 to 10:15 - **Davide Sangalli**
  First-Principles Carriers Dynamics Out of Equilibrium: a Many-Body Approach
- 10:15 to 10:40 - **Viktor Ivády**
  The Role of the Screening in the Density Functional Applied on Correlated Orbitals in an sp3 Electron Bath
- 10:40 to 11:00 - Coffee Break
- 11:00 to 11:25 - **Pedro Melo**
  A Unified Ab-initio Theory of Time-Resolved Photoluminescence within the Non-Equilibrium Green's Functions Approach
- 11:25 to 11:50 - **Lorenzo Sponza**
  Modifications of the Dielectric Response Evolving from Graphite to Graphene
- 11:50 to 12:15 - **Roberto Cardia**
  Angular and Compact Dibenzochrysene: the Role of Functionalizations on their Electronic and Optical Properties.
- 12:15 to 12:40 - **Igor Reshetnyak**
  New Starting Point for the Calculation of Optical Properties
- 12:40 to 14:20 - Lunch

Ground state

- 14:20 to 14:45 - **Xabier Zubizarreta Iriarte**
  Exchange Interaction and its Tuning in Magnetic Binary Chalcogenides
- 14:45 to 15:10 - **Sriram Poyyapakkam Ramkumar**
  Insights Into The Energetics of Cu2ZnSnS4: A Structural Perspective
- 20:00 to 22:00 - Social Dinner

Day 5 - May, 16th 2014

Ground state

- 10:00 to 10:25 - **Emanuele Coccia**
  Interplay between Geometry and Optical Properties in Biological Chromophores: Quantum Monte Carlo Ground State Structures for RPSB and Peridinin Molecules

- 10:25 to 10:50 - **Daniele Bovi**
  The S2 State of the Oxygen-Evolving Complex of Photosystem II Explored by QM/MM Dynamics: Spin Surfaces and Metastable States Suggest a Reaction Path towards the S3 State
- 10:50 to 11:15 - **Krisztian Szasz**
  Calculation of Hyperfine Tensor of Point Defects in Semiconductors
- 11:15 to 11:35 - Coffee Break
- 11:35 to 12:00 - Round Table Discussion: Future Directions
- 12:00 to 12:15 - Summary & Conclusions

Annex 4b: Full list of speakers and participants

Organisers

- Claudia Violante
- Olivia Pulci
- Lucia Reining
- Friedhelm Bechstedt
- Giovanni Ciccotti
- Adriano Mosca Conte
- Simone Melchionna
- Fernanda Lupinacci
- Matthieu Verstraete

Participants:

Belgium

- Andrés Rafael Botello Méndez
- Marco Di Gennaro
- Simon M.-M. Dubois
- Yannick Gillet
- Jonathan Laflamme Janssen
- Sriram Poyyapakkam Ramkumar

Finland

- Riku Tuovinen
- Anna-Maija Uimonen

France

- Yael Bronstein
- Elena Cannuccia **(invited speaker)**

- Sophie Chauvin
- Stefano Di Sabatino
- Carina Faber
- Nathaniel Raimbault
- Igor Reshetnyak
- Lorenzo Sponza
- Adrian Stan
- Nicolas Tancogne-Dejean
- Jianqiang Zhou

Germany

- Benjamin Buick **(invited speaker)**
- Wael Chibani
- Matteo Guzzo **(invited speaker)**
- Elham Khosravi **(invited speaker)**
- Linda Riele **(invited speaker)**
- Eugen Speiser **(invited speaker)**
- Andreas Stegmueller
- Falk Tandetzky **(invited speaker)**
- Adriano Violante **(invited speaker)**
- Xabier Zubizarreta Iriarte

Hungary

- Tamas Demjan
- Viktor Ivády
- Krisztian Szasz

Ireland

- Glenn Moynihan

Italy

- Matteo Barborini
- Daniele Bovi
- Roberto Cardia
- Emanuele Coccia
- Matteo Gerosa

- Micaela Matta
- Maria Montagna
- Davide Sangalli
- Stefano Schutzmann **(invited speaker)**
- Lorenzo Teodonio
- Daniele Varsano **(invited speaker)**
- Andrea Zen

Luxembourg

- Efterpi Kalesaki
- Alejandro Molina-Sánchez
- Henrique Pereira Coutada Miranda

Portugal

- Pedro Melo

United Kingdom

- Ryan McMillan
- Valerio Rizzi