Research Networking Programmes

Science Meeting – Scientific Report

Scientific report (one single document in WORD or PDF file) should be submitted online within two months of the event. It should not exceed seven A4 pages.

Proposal Title: *18th ETSF Workshop on Electronic Excitations: Applications to functional and energy materials*

Application Reference N°: 4611

Summary (up to one page)

The 18th ETSF Workshop on Electronic Excitations was held at the University of Luxembourg from the 1 to the 4 October. The focus of this year's workshop was the application of theoretical and computational spectroscopy to functional and energy materials. Specifically, the sections were dedicated to Spectroscopy of nanomaterials (nanotubes, nanowires, nanocrystals, bio-molecules), multiferroic materials (photo-ferroelectrics, magnetoelectric multiferroics, phase transitions in multiferroics), spectroscopy of photovoltaic materials, performance of novel xc-functionals for electronic excitations, electron-phonon coupling, and spectroscopy of defects. The sections were introduced by invited talks, experimental and theoretical. In total, there were 14 invited talks (speakers from Europe: France, Germany, Italy, Switzerland, Austria, Finland, Luxembourg; and USA) and 20 contributed talks. The poster session has been held on the Wednesday afternoon, counting about 50 contributions. Posters were displayed during the whole event to facilitate interactions among participants.

The workshop was attended by more than 100 participants, of which 70 young researchers. The participation of young researchers was actively encouraged by keeping the fee relatively low (400 euro of the fee including 4 nights in double room, coffee breaks, lunches and two dinners), by further allocating grants to young researchers, and by selecting their outstanding contributions for oral contributions.

Besides the funding from Psi-k/ESF, the workshop was co-financed by the Luxembourgish resesarch fund (FNR) and by the University of Luxembourg.

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

In the following, we give a description of the scientific presentations ordered by thematics rather than chronological order.

Photovoltaics:

A consistent part of the presentation and discussions was devoted to photovoltaics. More specifically to the understanding of electronic and optical properties of materials for photovoltaics and to the modelling of key processes such as charge transfer. Materials that received special attention, as they are very much investigated at the moment, were two dimensional graphene-like materials, such as few layers transition metal dichacolgenides, and chalcopyrites.

Photovoltaics based on two-dimensional graphene-like materials were the object of the invited contributions by M. Palummo. She demonstrated how first-principles calculations (Bethe-Salpeter equation) are a powerfool tool to investigate the electronic and optical properties of these materials and design new device architectures to efficiently implement photostable excitonic solar cells. Optical properties of two-dimensional materials calculated from first-principles were furthermore discussed in the two oral contributions by A. Molina-Sanchez and C. Attaccalite.

Defects on chalcopyrites, $Cu(In,Ga)Se_2$ and their relevance on electronic and optical properties were introduced from both the experimental and theoretical point of view. Susanne Siebentritt presented a review of the experimental methods to characterize defects, concentrating on photoluminescence spectroscopy. The number of shallow and deep impurity levels has changed over the years and is converging only very recently towards some agreement between the different groups. The unambiguous association the photoluminescence lines with particular point defects is still a challenge for theory. Risto Nieminen presented the progress of theory and computation in the determination of defect formation energies. The use of the HSE06 hybrid functional greatly improves the reliability of the calculations and leads to a reassignment of some of the defect levels in the band-gap with respect to earlier calcualtions on the level of the LDA or GGA approximations. The chemical potentials of the different constituent atoms enter the calculations as parameters. The exact values of these potentials depends on the experimental growth conditions whose simulation remains a considerable challenge.

Defects can be calculated in two different approaches: in the solid-state physics approach, large periodic supercells containing one point-defect are chosen and treated on the level of DFT and beyond. In the quantum-chemistry approach, the defect and the surrounding atoms are simulated as a large molecule embedded into an array of model potentials and/or point charges. A comparison of the two methods for the calculation of color centers in alkali halides was given in the invited talk by Peter Blaha. He showed that the GW+Bethe-Salpeter approach gives absorption energies in close agreement with wave-function methods such as CASPT2 (complete active-space perturbation theory of second order).

The modelling of charge transfer processes was a recurrent topic in several oral

contributions (F.P. Tiwald, I. Theophilou, P. Cudazzo, Z. Sun, P. V. Sushko). Charge transfer is not well captured in density-functional theory based approaches. However, wave-function based methods are too expensive to describe systems of interest for applications to energy materials. A solution was presented in the invited talk by Emily Carter. She proposed an embedding approach in which the charge transfer process is described by advanced wave-function methods, while the rest is modelled at density-functional level.

Thermoelectrics:

A second important strand of this year's conference, in the framework of functional materials and devices, was theoretical and experimental work on thermoelectric materials. Jeff Snyder is a seminal author in the field, having contributed many reviews and paradigm-setting articles. He presented some recent efforts to engineer the electronic band structure (the central quantity in our conference series) in order to couple more strongly electrical and thermal currents. Nanostructuring, alloying, and strain engineering are suggested as different avenues to increase the degeneracy of electronic bands near the effective Fermi level in doped semiconductors. The importance of more precise methods to access not only electronic states but also their variation in temperature was emphasized. The theme was compounded by Bin Xu, who presented a recent development in the fully ab initio calculation of the Seebeck coefficient, a notoriously delicate quantity which depends on electron energies, but also their lifetimes.

Design of novel materials for energy, genetic algorithms and high-throughput calculations:

In her invited talk Silvana Botti highlighted the importance of rigorous characterization of global structural properties of materials. This is important (a) to determine the ground state structure on which e.g. perform electronic/optical properties simulations (that is not always easy to determine experimentally as it was shown for p-type transparent conductive oxide $CuBO_2$); (b) To predict novel structure with some given property, as it was shown for various reconstruction of the α-boron (111) surface. The apparently prohibitive task of global structural minimization from ab-initio was performed by combining density-functional theory with a genetic algorithm.

A similar philosophy is followed in high-throughput calculations. Those calculations search for a material with a given property, rather than computing properties of a given material. The procedure combines data mining with database construction and density functional theory calculations. This relatively new but prolific field was represented by S. Curtarolo (invited) and G. Hautier (contributed). S. Curtarolo presented applications that cover several fields relevant to the conference topic such as photovoltaics, thermoelectricity and topological insulators. He stressed that in searching for materials with a given property it is key to define a suitable descriptor, a quantity with a defined physical meaning, though not necessarely an observable. G. Hautier showed application of the technique to p-type Transparent Conducting Oxides.

Multiferroics/Oxides

Open problems in multiferroics and complex oxides that can not be directly addressed

using standard ground-state electronic structure techniques but might be solvable with state-of-the art theoretical spectroscopies have been discussed by N. Spaldin in her invited talk. The invited talk of J. Kreisel focused on the experimental challenges related to the investigation of the intriguing phase diagram of multiferroics and anti-ferrroic materials, focusing especially on the multiple interacting mechanisms (electric polarity, octahedra rotations, magnetism and cooperative Jahn-Teller distortion) in $BiFeO_3$ and $BiMnO_3$. The "Multiferroics" session was completed by the contributed talks of Z. Zanolli (demonstrating electric control of magnetization in short-period $BiFeO_3/LaFeO_3$ superlattices) and P. Sushko (exploring how the optical properties of complex oxides can be modified in order to provide greater efficiency in capturing solar energy).

Electron-phonon coupling

The coupling of electrons and phonons (EPC) is central to many of the phenomena studied in this workshop. Matteo Calandra presented a very thorough invited review of EPC in different di-chalcogenide structures. These structures are extremely fashionable due to their 2D nature and similarities to graphene, but they also possess vibrational and superconducting properties which have presented a number of quandaries to experimentalists in understanding the charge (eventually spin) density waves they exhibit. The latter contribute to phase transitions and compete with other instabilities. In the particular case of $TiSe_2$,a contributed talk by Lucia Caramella contrasted the different possible explanations and origins for structural and electronic instabilities, leading to heated but cordial debate between the groups on the different approximations (exchange correlation, supercells, pseudopotentials) and their importance in representing the instabilities.

Y. Gilet presented a computational approach to the understanding of resonant Raman spectra of crystalline systems. He showed that excitonic effects may play a crucial role for some materials and have thus to be taken into account.

Finally, Andrea Marini presented a visionary work on the fundamentals of many-body perturbation theory and its clean extension to include vibrational effects. He showed that the good agreement of phonon frequencies calculated by density functional perturbation theory (DFPT) with experiment is probably the result of consistently neglecting certain types of electronic screening in appropriate parts of the propagators and vertices for many-body diagrams coupling electrons and phonons to higher order. He presented consistent and practical rules for employing DFPT quantities in expressions involving higher order diagrams, in order to avoid double-screening effects.

Large systems:

Research in novel materials for energies usually addresses complex and relatively large systems. It is then essential to devise suitable approaches and algorithms. The invited talk of Gabriel Bester tackled the problem by presenting an approach to treat optical properties for systems with thousands of atoms. He made the connection between density-functional theory based approaches and configuration interaction in quantum chemistry. He thus showed that it is possible to obtain from ab-initio optical properties of quantum dots and at the same time have the necessary accuracy to treat atomic defects. Two contributed talks (D. Rocca and Mathias Ljungberg) presented improved

algorithms for solving the Bethe-Salpeter equation showing as well interesting applications to third generation photovoltaics materials.

Developement of methods:

Georg Kresse presented a talk on recent implementations of wave-function methods in the VASP code. While standard DFT is very efficient and probably accurate enough for an estimated 80% of computational applications, it can fail dramatically for the remaining 20% of problems. Many-body extensions of DFT such as total-energy calculations on the level of the random-phase approximation (RPA) have made a lot of progress for the calculation of cohesion energies. The latest development in VASP is the implementation of a wave-function method, full configuration interaction quantum Monte Carlo. This has been applied to a variety of real solids and provide new reference total energies for the testing of a variety of “cheaper” methods.

Guido Fratesi presented a new way to investigated charge transfer between a molecule and a metallic surface by means of a non-equilibrium approach similar to the one used in quantum transport. He presented promising results that compared very well with the experiments .

Standards and software development

Finally we would to mention the ETSF software meeting. During this meeting developers of different computational codes had the opportunity to exchange views about new standards for data interchange, and new way to develop common libraries. Regarding this last point there were several discussions on the new developments in the exchange-correlation library (LibXC) and the pseuso-potential library (Libpspio),

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

Results emerging from the conference are very positive. Several works there presented showed clearly that computational spectroscopy methods significantly contribute to the research area of energy and functional materials. Their contribution is essential in connecting optical, structural and electronic structure properties of materials. Being capable of capturing many-body effects, they can uncover subtle, but important mechanisms and therefore inspire new experiments and possible applications. A nice example of the predicting power of state-of-the-art calculation was given e.g. in the work presented by Maurizia Palummo on two-Dimensional Materials for ultrathin optoelectronic devices. A second important example, in a different direction, it is the possibility to design new materials with desired properties through high-throughput calculations by using he set of tools from electronic structures in combination with other tools (data-mining, genetic algorithms) as it has been shown in the seminar of Stefano Curtarolo.

The conference also showed that the research area of energy and functional materials poses serious challenges to the computational spectroscopy community stimulating development of new approaches and refinement of existing one. Challenges are both computational/numerical, regarding the size of the systems (number of atoms), their complexity (e.g. defects, interfaces that break the translational symmetry); and theoretical, as for example for the charge-transfer problem that was mentioned earlier.

What clearly emerges from many of the presented works and discussions is that the challenges posed by research in energy and functional materials requires a synergy of methodologies to be tackled. It is therefore important for the community to make contact with other communities, learn their methodologies and try to merge different approaches. In this perspective, the conference was designed to showcase highlights and open problems not only from the particular area of computational spectroscopy, but also from neighbouring areas and from related experimental research. This provided a fertile basis for discussions on common problems in different areas and how methods from different areas can concur in tackling particular problems.

We believe thus that the direction those discussions indicated is that besides the improvement of algorithms and of the accurateness of the available methods, development of multiscale or embedding techniques that bridge between different level of theory will be essential for applications to energy and functional materials. Nice examples of the possibilities offered by such approaches were given in the talk of Emily Carter and Gabriel Bester.

Annex 4a: Programme of the meeting

Day	Monday 30 September
14:00	**Nanoquanta Steering Committee meeting**
16:00	**MB infrastructure**
18:00	**ETSF Software meeting**
19:30	Welcome drink and dinner
Day	Tuesday 1 October
9:00	Registration and Opening
9:15	Towards an exact description of the many electron wavefunction in solids: ful CI and coupled cluster **Georg Kresse**
10:00	First-principles study of excitonic effects in Raman intensities **Yannick Gillet**
10:20	Coffee Break
10:50	Carrier Pocket Engineering to Improve Thermoelectric Transport **Jeff Snyder**
11:35	Fast electron transfer at molecule-substrate interfaces **Guido Fratesi**
11:55	Nonlinear optics by means of modern theory of polarization **Claudio Attaccalite**
12:15	Lunch
14:15	The F-center in LiF **Peter Blaha**
15:00	Ab-initio approach to the charge transfer during scattering of a proton from a LiF surface **Franz Paul Tiwald**
15:20	Calculations of Near Edge Absorption Fine Structure (NEXAFS) of phthalocyanines adsorbed on metallic substrates: FePc/Co(001) and FePc/O/Co(001) **Barbara Brena**
15:40	Coffee Break
16:10	Exciton dynamics in carbon nanotubes **Tobias Hertel**

17:00	**ETSF general meeting**
17:45	**User projects meeting**
Day	Wednesday 2 October
9:00	Designing and understanding novel materials for energy **Silvana Botti**
9:45	Two-Dimensional Materials for ultrathin optoelectronic devices **Maurizia Palummo**
10:30	Coffee Break
11:10	Exciton dissociation into free charge carriers in donor-acceptor polymer heterojunctions **Zhen Sun**
11:30	Climbing up the BBGKY hierarchy: Curing the divergence problem with a new approximation **Javad Hashemi**
11:50	Charge transfer excitations from Hartree-Fock subsequent minimization scheme **Iris Theophilou**
12:10	Second Order Cumulant Expansion for the Electron Green's Function **Joshua Kas**
12:30	Lunch
14:30	The high-throughput highway to computational materials design **Stefano Curtarolo**
15:15	First Principles explanation of the positive Seebeck coefficient of lithium **Bin Xu**
15:35	Efficient solution of the Bethe-Salpeter equation in a local basis **Mathias Ljunbberg**
15:55	Coffee Break
16:35	Defects in chalcopyrites **Susanne Siebentritt**
17:30	**Poster session** (with finger food)
Day	Thursday 3 October
9:00	Defect physics of chalcopyrite solar-cell materials: insight from first-principles calculations **Risto Nieminen**

9:45	Charge Transfer Excited States from First Principles Theories **Emily Carter**
10:30	Coffee Break
11:05	Calculation of the optical properties of large nanostructures and atomic defects using a configuration interaction approach **Gabriel Bester**
11:50	Computational spectroscopy using many-body perturbation theory: Large scale calculations without virtual orbitals **Dario Rocca**
12:10	Frenkel versus charge-transfer exciton dispersion in molecular crystals **Pierluigi Cudazzo**
12:30	Lunch
14:30	Why I would like to be able to do theoretical spectroscopy **Nicola Spaldin**
15:15	Electric control of the magnetization in BiFeO3/LaFeO3 superlattices **Zeila Zanolli**
15:35	Character of the optical transitions in strained LaCrO3, LaFe(1–x)CrxO3 and (Fe(1–x)Crx)2O3 solid solutions studied using an embedded cluster method **Peter Sushko**
15:55	Coffee Break
16:30	Intriguing phases and phase transitions in Bi-based ABO3-type multiferroics **Jens Kreisel**
17:15	Identification of Low Hole Effective Mass Novel p-type Transparent Conductir Oxides by High-Throughput Computing **Geoffroy Hautier**
18:00	Visit to Luxembourg city
20:00	Social Dinner
Day	Friday 4 October
9:00	Superconductivity and charge density wave in metallic transition metal dichalchogenides. **Matteo Calandra**
9:45	Phonon softening and structural instabilities in TiSe2 **Lucia Caramella**
10:05	Effect of spin-orbit interaction on the excitonic effects in single-layer,

	double-layer, and bulk MoS2 **Alejandro Molina-Sanchez**
10:25	Coffee Break
11:00	A new formulation of the the Many-Body approach to the electron-phonon problem in realistic materials **Andrea Marini**
11:20	A critical assesment of the Tamm-Dancoff Approximation in Reproducing Vibronic Absorption and Emission Band Shapes **Agisilaos Chantzis**
11:40	Closing Remarks
12:00	Lunch

Annex 4b: Full list of speakers and participants

Full list of speakers

Georg Kresse
Yannick Gillet
Jeff Snyder
Guido Fratesi
Claudio Attaccalite
Peter Blaha
Franz Paul Tiwald
Barbara Brena
Tobias Hertel
Silvana Botti
Maurizia Palummo
Zhen Sun
Javad Hashemi
Iris Theophilou
Joshua Kas
Stefano Curtarolo
Bin Xu
Mathias Ljunbberg
Susanne Siebentritt
Risto Nieminen
Emily Carter
Gabriel Bester
Dario Rocca
Pierluigi Cudazzo
Nicola Spaldin
Zeila Zanolli
Peter Sushko
Jens Kreisel
Geoffroy Hautier
Matteo Calandra
Lucia Caramella
Alejandro Molina-Sanchez
Andrea Marini
Agisilaos Chantzis

Full list of participants

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Frederique Bertrand, University of Luxembourg (Luxembourg)
Gabriel Bester, Max Planck Institute Stuttgart, FKF (Germany)
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