Research Networking Programmes

Science Meeting – Scientific Report

Proposal Title: **HoW exciting! Hands-on Workshop on Excitations in Solids 2014**

Application Reference N°: 5266

1) Summary

The "HoW exciting! 2014" hands-on workshop combined keynote lectures giving an introduction to theoretical foundations for the calculation of excitations in solids with hands-on exercises using the software package **`exciting`**. The workshop took place at the campus Adlershof of the Humboldt-Universität zu Berlin from July 31 to August 8, 2014. The CECAM workshop was the third event in a series after the very successful workshops, which took place in November 2010 in Lausanne, Switzerland, and in August 2012 in Berlin, Germany. The participants enjoyed a varied programme of interesting lectures, hands-on exercises and discussions. It turned out to be very successful and reached all the expected goals.

Web pages:

http://www.cecam.org/workshop-1071.html
http://how-exciting-2014.physik.hu-berlin.de

Notes of the lectures presented at the workshop can be found as PDF files at the following link:

http://exciting-code.org/how-exciting-2014-hands-on-workshop-berlin

The list and description of the tutorial exercises is also available at:

http://exciting-code.org/tutorials-boron

2) Description of the scientific content of and discussions at the event

The first day of the workshop was dedicated to the foundations of density-functional theory (DFT) and augmented plane-waves (APW) methods, with the keynote lectures by Kieron Burke and Andris Gulans. In the talk by Burke, the main ingredients of DFT were presented and discussed, including the Hohenberg-Kohn theorems, the Kohn-Sham scheme, and the most common approximations for the exchange-correlation (xc) energy functional. Andris Gulans presented DFT in the flavor of the full-potential, all-electron APW scheme, as implemented in the **exciting** code. The main characteristics of this approach were presented, in close connection with the code structure. The tutorial talk by Pasquale Pavone presented an introduction to **exciting**, showing an overview of properties that can be computed with this code. The following lab session was dedicated to familiarize with the code and with the computational parameters which mainly impact of the results obtained with **exciting**. Convergence studies of the influence of the k-points sampling and the size of the basis set were performed in the following hands-on tutorial.

The second day of the workshop was dedicated to electronic properties and structural optimization. Kieron Burke gave the morning keynote lecture, presenting the main open issues related to DFT, which may affect crucially the description of the electronic properties of materials at the mean-field level. The tutorial talk by Jürgen Spitaler introduced electronic-structure calculations in **exciting**. In the hands-on session, the participants used **exciting** to calculate the electronic properties (band structure, density of states, and Kohn-Sham wave-functions) of prototypical metallic and semiconducting materials. In the afternoon lecture, Jorge Sofo talked about graphene, which is extremely sensitive to geometrical modifications and distortions. In the following tutorial talk, Pasquale Pavone presented the approaches implemented in **exciting** to perform structural optimization and atomic relaxation. In the hands-on session the participants put their knowledge into practice, using **exciting** to optimize and relax different crystal structures (simple cubic, wurzite, etc.) and simple molecules. In the evening the poster session took place. About 15 participants presented their posters in a scientifically stimulating and lively atmosphere.

On the third day, Lucia Reining presented the foundations of theoretical spectroscopy, with specific focus on time-dependent DFT (TDFFT). The tutorial talk by Santiago Rigamonti introduced the implementation of TDDFT in **exciting**. In the lab session, the students performed a basic TDDFT calculation for the loss function of bulk silver in the long-wavelength limit. In the afternoon session, Miguel Marques gave a keynote lecture about xc functional, explaining their main features and their applicability to different kind of materials. He introduced hybrid functionals, which have been the subject of an intense research in recent years. These topics were further explained and discussed in the tutorial talk by Ute Werner, who explained how hybrid functionals are implemented in **exciting**. She also introduced the library of xc functionals **libxc**, which is supported by **exciting**. During the following tutorial session participants could use the **libxc** to calculate the optimal volume and bulk modulus of silicon. Students could also learn how to perform band-structure calculations using hybrid functionals, in the flavor of optimized effecitve potential - exact-exchange method by calculating the band-structure of diamond. During the lab session post-processing tools to include Van der Waals corrections to the total energy of graphite were also introduced, in order to find the equilibrium interlayer separation and the corresponding binding energy.

The fifth day started with the keynote lecture by Mark van Schilfgaarde about *GW* methods. He introduced the Green's functions formalism in theoretical spectroscopy,

presenting an overview of this approach ranging from the simplest approximations (e.g. COHSEX), to the conventional G_0W_0 approach, up to the most sophisticated self-consistent methodologies. In the tutorial session, Dmitrii Nabok introduced the implementation of G_0W_0 in **exciting**. In the hands-on tutorial, the participants could compute the electronic structure of bulk silicon by applying G_0W_0. In the afternoon session, Lucia Reining presented the Bethe-Salpeter Equation (BSE) approach to compute optical spectra in solids, including explicitly the electron-hole interaction. In the tutorial talk, Caterina Cocchi presented the implementation of BSE in **exciting**, introducing the main parameters in the code. In the lab session, participants could put their knowledge into practice, by computing the BSE absorption spectrum of lithium fluoride using **exciting**. They could also investigate the behavior of different TDDFT kernels, which explicitly include many-body effects, also applied to lithium fluoride.

The first part of the sixth day was dedicated to phonons and electron-phonon coupling. Miguel Marques presented the topic in his keynote lecture, focusing especially on the formalism of density-functional perturbation theory (DFPT). He introduced the main concepts and formulas behind DFPT and presented some results showing the importance of electron-phonon coupling in the properties of insulators, semiconductors and superconducting materials. The frozen-phonon approach, as implemented in **exciting**, was discussed in details in Karsten Hannewald's tutorial talk. In the hands-on session, participants calculated the phonon-dispersion curves of diamond, as prototypical material. In the afternoon, Silvana Botti gave a keynote lecture about advances in many-body perturbation theory (MBPT). She presented some recent results about photovoltaic materials, where many-body effects play a crucial role. Examples of these materials are kesterites, which are promising light-harvesting compounds. The tutorial talk by Weine Olovsson was focused on X-ray absorption spectroscopy (XAS), computed within **exciting** in the framework of MBPT. He showed that core-level excitations can accurately be described by explicitly including the electron-hole interaction, as in the BSE formalism. In the lab session afterward, the students could use the BSE package of **exciting** to compute XAS of prototypical materials such as lithium fluoride and cubic boron nitride.

On the seventh day of the workshop, the first keynote lecture was given by Clas Persson, who discussed the recent theoretical advances about solar cells. The tutorial session was dedicated to Raman spectroscopy, introduced by Stefan Kontur in his talk. He presented newly implemented routines that allow to calculate Raman spectra with **exciting**. In the lab session, participants could use the code to compute the Raman spectrum of bulk silicon. In the same hands-on session, another tutorial was presented, concerning the calculation of thermal-expansion coefficient, as well as the mode Grüneisen parameters of diamond. In the afternoon session, Jorge Sofo gave a plenary talk on thermoelectric materials, introducing the main formalism to compute thermoelectric properties from first-principles. The tutorial session was introduced by Rostam Golesorkhtabar, who presented the package **ElaStic**, which is interfaced to **exciting** for the calculation of elastic constants in any crystal structure. In the lab session the participants could use this tool to compute the elastic constants of diamond and of beryllium in the hexagonal crystal phase. In the same session, students used **exciting** to compute ground-state energy of strained materials and the derivatives of the energy-vs-strain curves at zero strain. They could learn how these quantities are related to elastic constants. They also computed the full stress tensor of hexagonal beryllium, as a prototypical example. The second part of the tutorial session was dedicated to spin-polarized calculations, including spin-orbit coupling. As an example, participants focused on the ground-state properties of iron, with different types of magnetic order.

The morning session of the eighth day started with the keynote lecture by Christian Carbogno about heat transport. He presented the formalism and showed results about zirconia. The tutorial session was introduced by Santiago Rigamonti, who presented the magneto-optical Kerr effect (MOKE) and its implementation in **exciting**. He also showed how to obtain scanning-tunneling-microscopy (STM) spectra with **exciting**. Participants could use the **exciting** code to compute MOKE on nickel and the STM spectrum of tungsten. In the afternoon, Anton Kozhevnikov gave a keynote lecture about **SIRIUS**, a parallel library interfaced to **exciting**, which allows to efficiently compute ground-state properties of huge systems (>1000 atoms).

The last day of the workshop hosted only one keynote lecture, about big data analysis, given by Matthias Scheffler. He showed the state-of-the-art approaches to treat big data and to predict properties from them.

The last two lab sessions were dedicated to users' projects. The high level of the participants contributed to stimulate lively scientific discussions. Calculations of excited-state properties using GW and BSE approaches, core level excitations and phonons were among the most discussed themes. Most of the participants used **exciting** to treat their own systems of interests, ranging from bulk magnetic materials, to two-dimensional heterostructures, to single molecules.

3) Assessment of the results and impact of the event on the future directions of the field

"HoW exciting! 2014" received a very positive feedback from the participants, as indicated by the analysis of a survey delivered to them on the last conference day. There were a total of 70 scientific participants, among them 5 organisers, 21 lecturers, 6 tutors, and 38 students from institutions of 18 countries, including several European nations, Algeria, Canada, Israel, Malaysia, Singapore and the USA.

Almost all the participants declared themselves very satisfied (66%) or satisfied (33%) with the workshop. In particular, they all judged good or very good the scientific program of the workshop overall, as well as the keynote lectures given by the invited speakers, the hands-on tutorial sessions lead by the members of the **exciting** team, and the **exciting** tutorial web pages. Significantly, most participants (91%) considered "HoW exciting! 2014" as an important or very important experience for their future career.

Concerning the dissemination of the code, 94% of the participants declared to be willing to use **exciting** in their research activity. Considerable interest has been demonstrated for the packages to compute optical properties and many-body perturbation theory (GW approximation and the Bethe-Salpeter equation). The features related to the all-electron implementation of density functional theory, as developed in exciting, including LAPW approaches and calculation of X-ray absorption spectra also attracted the attention of almost one half of the participants. They also manifested their interest in the calculation of vibrational properties, in the flavor of phonons and elastic constants, as well as Raman spectra.

Significant consideration has been devoted also to the soon available features of exciting, including its portability to high performance computing architectures. In addition, the largest majority of the participants, including undergraduate and graduate students as well as post-docs, expressed interest in future collaborations with the **exciting** team.

In order to reach the broadest audience and to update the user community with the newest feature of the **exciting** code, we believe it is appropriate to keep the schedule of a "HoW exciting!" tutorial every second year.

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

Annex 4a: Programme of the meeting

Day 1 - July 31, 2014

14:00 - 14:15	*Opening*	
14:15 - 15:15	Kieron Burke	*DFT I*
15:15 - 16:15	Andris Gulans	*APW*
16:15 - 16:45	Pasquale Pavone	*Getting started*
16:45 - 17:00	*Coffee break*	
17:00 - 19:00	*Exercises:*	*How to converge ground-state calculations*
19:00	*Dinner*	

Day 2 - August 1, 2014

09:00 - 10:00	Kieron Burke	*DFT II*
10:00 - 10:30	Jürgen Spitaler	*Electronic structure*
10:30 - 10:45	*Coffee break*	
10:45 - 12:45	*Exercises:*	*Electronic structure and state visualization*
12:45 - 14:15	*Lunch break*	
14:15 - 15:15	Jorge Sofo	*Graphene*
15:15 - 15:45	Pasquale Pavone	*Structure optimization*
15:45 - 16:00	*Coffee break*	
16:00 - 18:30	*Exercises:*	*Optimization and molecules*
18:30	*Dinner*	
20:30	*Poster Session*	

Day 3 - August 2, 2014

09:00 - 10:00	Lucia Reining	*TDDFT*
10:00 - 10:30	Santiago Rigamonti	*Practical aspects of TDDFT calculations*
10:30 - 10:45	*Coffee break*	
10:45 - 12:45	*Exercises:*	*TDDFT*
12:45 - 14:15	*Lunch break*	
14:15 - 15:15	Miguel Marques	*Exchange correlation (xc) functionals*
15:15 - 15:45	Ute Werner	*Using xc functionals in \exciting*
15:45 - 16:00	*Coffee break*	

16:00 - 18:30	*Exercises:*	*xc functionals, exact exchange, and van-der-Waals functionals*
18:30 - 20:00	*Dinner*	

Day 4 - August 3, 2014

Excursion
Social dinner

Day 5 - August 4, 2014

09:00 - 10:00	Mark van Schilfgaarde	*GW*
10:00 - 10:30	Dmitrii Nabok	*Practical aspects of GW calculations*
10:30 - 10:45	*Coffee break*	
10:45 - 12:45	*Exercises:*	*GW*
12:45 - 14:15	*Lunch break*	
14:15 - 15:15	Lucia Reining	*Many-body perturbation theory I*
15:15 - 15:45	Caterina Cocchi	*Bethe-Salpeter Equation (BSE)*
15:45 - 16:00	*Coffee break*	
16:00 - 18:30	*Exercises:*	*BSE*
18:30	*Dinner*	

Day 6 - August 5, 2014

09:00 - 10:00	Miguel Marques	*Electron-phonon coupling*
10:00 - 10:30	Karsten Hannewald	*Phonons*
10:30 - 10:45	*Coffee break*	
10:45 - 12:45	*Exercises:*	*Phonons*
12:45 - 14:15	*Lunch break*	
14:15 - 15:15	Silvana Botti	*Many-body perturbation theory II*
15:15 - 15:45	Weine Olovsson	*X-ray scattering*
15:45 - 16:00	*Coffee break*	
16:00 - 18:30	*Exercises:*	*X-ray scattering*
18:30	*Dinner*	

Day 7 - August 6, 2014

09:00 - 10:00	Clas Persson	*Solar energy*

10:00 - 10:30	Stefan Kontur	*Raman spectra*
10:30 - 10:45	*Coffee break*	
10:45 - 12:45	*Exercises:*	*Raman spectra and thermal expansion*
12:45 - 14:15	*Lunch break*	
14:15 - 15:15	Jorge Sofo	*Thermoelectrics*
15:15 - 15:45	Rostam Golesorkhtabar	*Elastic constants*
15:45 - 16:00	*Coffee break*	
16:00 - 18:30	*Exercises:*	*Elastic constants with* ***ElaStic*** *and spin-polarization*
18:30	*Dinner*	

Day 8 - August 7, 2014

09:00 - 10:00	Christian Carbogno	*Thermal conductivity*
10:00 - 10:30	Santiago Rigamonti	*Magneto-optic Kerr effect (MOKE)*
10:30 - 10:45	*Coffee break*	
10:45 - 12:45	*Exercises:*	*MOKE + STM*
12:45 - 14:15	*Lunch break*	
14:15 - 15:15	Anton Kozhevnikov	*SIRIUS: a large scale parallelization project*
15:15 - 15:30	*Coffee break*	
15:30 - 18:30	*User projects*	
18:30	*Dinner*	

Day 9 - August 8, 2014

09:00 - 10:00	Matthias Scheffler	*NoMaD: Novel Materials' Discovery*
10:00 - 10:15	*Coffee break*	
10:15 - 12:45	*User projects*	
12:45 - 13:00	*Closure*	
12:45 - 14:15	*Lunch*	

Annex 4b: Full list of speakers and participants

ORGANISERS:

Pasquale Pavone	*Humboldt-Universität zu Berlin, Germany*
Caterina Cocchi	*Humboldt-Universität zu Berlin, Germany*
Giulio Biddau	*Humboldt-Universität zu Berlin, Germany*
Claudia Draxl	*Humboldt-Universität zu Berlin, Germany*
Jürgen Spitaler	*Materials Center Leoben Forschung GmbH, Austria*

LECTURERS:

Silvana Botti	*CNRS and University of Lyon, France*
Kieron Burke	*University of Calithium fluorideornia Irvine, USA*
Christian Carbogno	*FHI Berlin, Germany*
Caterina Cocchi	*Humboldt-Universität zu Berlin, Germany*
Rostam Golesorkhtabar	*Humboldt-Universität zu Berlin, Germany*
Andris Gulans	*Humboldt-Universität zu Berlin, Germany*
Karsten Hannewald	*Humboldt-Universität zu Berlin, Germany*
Stefan Kontur	*Humboldt-Universität zu Berlin, Germany*
Anton Kozhevnikov	*CSCS, Switzerland*
Miguel Marques	*University of Lyon, France*
Dmtrii Nabok	*Humboldt-Universität zu Berlin, Germany*
Weine Olovsson	*Linköping University, Sweden*
Pasquale Pavone	*Humboldt-Universität zu Berlin, Germany*
Clas Persson	*University of Oslo, Norway*
Lucia Reining	*CNRS Palaiseau and Ecole Polytechnique, France*
Santiago Rigamonti	*Humboldt-Universität zu Berlin, Germany*
Matthias Scheffler	*FHI Berlin, Germany*
Mark van Schilfgaarde	*Kings College London, UK*
Jorge Sofo	*Penn State Unviersity, USA*
Jürgen Spitaler	*Materials Center Leoben, Austria*
Ute Werner	*Humboldt-Universität zu Berlin, Germany*

TUTORS:

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Nora Salas Illanes	*Humboldt-Universität zu Berlin, Germany*
Kathrin Glantschnig	*University of Leoben, Austria*
Olga Turkina	*Humboldt-Universität zu Berlin, Germany*

STUDENT PARTICIPANTS:

Adela Nicolaev	*University of Bucharest, Faculty of Physics, Romania*
Albin Hertrich	*Humboldt-Universität zu Berlin, Germany*
Archana Manoharan	*Humboldt-Universität zu Berlin, Germany*
Bakhtiar Ul Haq	*University Teknologi, Malaysia*
Benjamin Aurich	*Humboldt-Universität zu Berlin, Germany*
Bernhard Klett	*Humboldt-Universität zu Berlin, Germany*
Celso Ricardo Caldeira Rêgo	*Instituto de Física de São Carlos-University of São Paulo, Brazil*
Estelina Lora da Silva	*University of Bath, United Kingdom*
Evan Laksono	*National University of Singapore, Singapore*
Evgeny Blokhin	*Humboldt-Universität zu Berlin, Germany*
Fairoja Cheenicode Kabeer	*University of Kassel, Germany*
Felix Kramer	*Humboldt-Universität zu Berlin, Germany*
Hussien Osman	*Oviedo University, Spain*
Jens Wehner	*Max Planck Institute for Polymer Research, Germany*
Jin Wen	*Academy of Sciences, Czech Republic*
Jonathan Skelton	*University of Bath, United Kingdom*
Jos Boschker	*Paul-Drude-Institut, Germany*
Jose David Cojal Gonzalez	*Humboldt-Universität zu Berlin, Germany*
Jose Lado	*INL, Portugal*
Joseph Gonzalez	*University of South Florida, USA*
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Juan Fernández Afonso	*University of Santiago de Compostela, Spain*
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Ronaldo Pela	*Technolical Institute of Aeronautics , Brazil*
Sven Lubeck	*Humboldt-Universität zu Berlin, Germany*
Torsten Wendav	*Humboldt-Universität zu Berlin, Germany*
Vijay Singh	*Post-Doctoral Fellow, Israel*
Vladimir Zobac	*Academy of Sciences of the Czech Republic*
Wahib Aggoune	*University A. Mira of Bejaia, Algeria*