Report on Workshop:

HoW exciting!
Hands-on Workshop on Excitations in Solids 2012

Humboldt Universität zu Berlin, Germany

August 2-8, 2012

Sponsors:

CECAM, Psi-k

Organisers:

Claudia Ambrosch-Draxl - Humboldt Universität zu Berlin
Pasquale Pavone - Humboldt Universität zu Berlin
Jürgen Spitaler - Materials Center Leoben Forschung GmbH

Web pages:

`http://www.cecam.org/workshop-0-776.html`
`http://exciting-code.org/how-exciting-2012`

Summary

The CECAM workshop was devoted to the presentation of both theoretical concepts and computational tools (embedded in the software package **`exciting`**) that are needed for the calculations of various excitations in solids. The workshop took place at the Humboldt Universität zu Berlin in August 2012. It turned out to be very successful and reached all the expected goals. The participants enjoyed a varied programme of interesting lectures and discussions. The CECAM workshop was the second event in a series after the very successful workshop "HoW exciting! Hands-on workshop on excitations in solids employing the **`exciting`** code" taking place in Nov. 2010, in Lausanne, Switzerland.

Workshop background

Density-functional theory (DFT) has proven to be an excellent technique for the calculation of structures and molecular dynamics such that a variety of popular DFT codes has already been established for being used by a large and even swiftly growing community. While most of the applications are still dedicated to the investigation of ground-state properties, there is rapidly increasing demand for understanding and predicting various kinds of excitations. The topics range from light-matter interaction via spin fluctuations, lattice vibrations and distortions, to situations where several fundamental excitations take place on the same energy scale and may interact with each other.

This scenario gives raise to many exciting basic scientific questions which, at the same time, are important in terms of industrial applications. While light- or current-induced electronic excitations play the major role in opto-electronic devices, lattice excitations and their interaction with the electronic system lead to phenomena like superconductivity or the thermal behaviour of materials. All these effects are extremely relevant in industrial products such as solar cells, light-emitting diodes, and high-strength materials or thermal coatings. Such considerations require the development of basic concepts as well as the corresponding computer codes capable of dealing with these situations.

Workshop contents

The CECAM workshop provided training of young people, making them familiar with the **`exciting`** code, a package which is dedicated to excited-state properties.

Besides the fundamentals related to the method (Draxl, Gulans, Golesorkhtabar, Meisenbichler, Nabok, Pavone, Olovsson, Spitaler, Werner) and hands-on exercises, we had keynote lectures given by world-leading experts in the various fields. They comprised the cornerstones of DFT (Burke), time-dependent DFT (Gross), many-body perturbation theory and GW (Hybertsen and Rinke), linear-response theory and phonons (Baroni), recent discoveries on graphene-like materials and thermoelectrics (Sofo), and future perspectives for the field (Rubio).

By exploring the fundamental physical concepts in combination with practical exercises, the participants could profit from another exciting experience, which is learning by doing.

The exciting code

The simulation package **exciting** (web site: `http://exciting-code.org`) is a young public-domain all-electron package based on DFT for the investigation of condensed matter on the atomic scale. It combines several major advantages:

- It is a full-potential all-electron code based on the linearized augmented plane-wave (LAPW) method, which stands for highest precision and the fact that it can be used for any material.
- It is the only all-electron package comprising vast implementations of excited state properties within TDDFT as well as many-body perturbation theory.
- It is developers-friendly through a clean and fully documented programming style, being written from scratch and handled with a modern version-control system (git).
- It is user-friendly through an easy-to-handle user interface comprising various tools to create and validate input files and analyze results.
- It is powerful through the use of xml, which enables users to do extremely efficient scripting and to design complex computational experiments with minimal effort.
- It is seminal by being interfaced to packages operating on the next higher length scale and by the development of tools which allow for the handling by users from an industrial environment.

Notes and statistics

Notes of the lectures presented at the workshop can be found as PDF files at the web page `http://exciting-code.org/cecam-talks-2012`. The list and description of the tutorial exercises is also available at `http://exciting-code.org/tutorials`.

There were a total of 53 scientific participants, among them 3 organisers, 7 lecturers, 12 tutors, and 31 student participants from institutions of 15 countries, including various European nations, Japan, Taiwan, India, Algeria, Tunisia and the USA.

Reception by the participants

After the workshop, we received a very positive feedback from the student participants showing that they enjoyed very much this tutorial. In particular, they found the workshop very nice and well organized and were enthusiastic about both the pedagogical and scientific quality of all lecturers. The competence and availability of the tutors during the exercises was also very much appreciated.

Pictures of the workshop

Programme

Day 1 - August 2, 2012

08:45 - 09:00	Opening
09:00 - 10:00	**Kieron Burke** *DFT I*
10:00 - 10:30	**Pasquale Pavone** *Getting Started*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *Basics, I/O, running & convergence studies*
12:45 - 14:15	Lunch Break
14:15 - 15:15	**Claudia Draxl** *LAPW*
15:15 - 16:30	Exercises: *Electronic structure*
16:30 - 16:45	Coffee Break
16:45 - 18:00	Exercises: *EOS*
18:00 - 19:00	**Jorge Sofo** *Graphene*
19:00 - 20:30	Wine, cheese, & more

Day 2 - August 3, 2012

09:00 - 10:00	**Kieron Burke** *DFT II*
10:00 - 10:30	**Rostam Golesorkhtabar** *Elastic properties*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *Elastic constants*
12:45 - 14:15	Lunch Break
14:15 - 15:15	**E.K.U. Gross** *TDDFT I*
15:15 - 15:45	**Ute Werner** *XC functionals*
15:45 - 16:00	Coffee Break
16:00 - 18:00	Exercises: *XC & spin*

Day 3 - August 4, 2012

09:00 - 10:00	**Mark Hybertsen** *GW I*
10:00 - 10:30	**Dmitrii Nabok** *GW@exciting*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *GW*
12:45 - 14:15	Lunch Break
14:15 - 15:15	**E.K.U. Gross** *TDDFT II*
15:15 - 15:45	**Claudia Draxl** *Optical excitations*
15:45 - 16:00	Coffee Break
16:00 - 18:00	Exercises: *Excited states with TDDFT & q-dependent TDDFT*

Day 4 - August 5, 2012

Excursion

Day 5 - August 6, 2012

09:00 - 10:00	**Mark Hybertsen** *GW II*
10:00 - 10:30	**Weine Olovsson** *Core spectroscopy*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *BSE & core levels*
12:45 - 14:15	Lunch Break
14:15 - 15:15	**Patrik Rinke** *GW II*
15:15 - 15:45	**Jürgen Spitaler** *Complex systems*
15:45 - 16:00	Coffee Break
16:00 - 18:00	Exercises: *ATAT@exciting & ASE@exciting & surfaces*

Day 5 - August 6, 2012

09:00 - 10:00	**Stefano Baroni** *LRT I*
10:00 - 10:30	**Pasquale Pavone** *Phonons*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *Phonons & thermal properties*
12:45 - 14:15	Lunch Break
14:15 - 15:15	**Stefano Baroni** *LRT II*
15:15 - 15:45	**Hong Li** **exciting***@web*
15:45 - 16:00	Coffee Break
16:00 - 18:00	Exercises: **exciting***@web*

Day 7 - August 8, 2012

09:00 - 10:00	**Jorge Sofo** *Thermoelectrics*
10:00 - 11:15	Panel discussion
11:45 - 12:00	Coffee Break
12:00 - 13:00	**Angel Rubio** *Perspectives*

List of participants

Organisers

Claudia Draxl	Humboldt Universität zu Berlin, DEU
Pasquale Pavone	Humboldt Universität zu Berlin, DEU
Jürgen Spitaler	Materials Center Leoben, AUT

Lecturers

Stefano Baroni	International School for Advanced Studies, Trieste, ITA
Kieron Burke	University of California Irvine, USA
E.K.U. Gross	Max Planck Institute of Microstructure Physics, Halle, DEU
Mark Hybertsen	Brookhaven National Laboratory, USA
Patrik Rinke	Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, DEU
Angel Rubio	Universidad del País Vasco, San Sebastian, ESP
Jorge Sofo	Pennsylvania State University, State College, USA

Tutors

Rostam Golesorkhtabar	Humboldt Universität zu Berlin, DEU
Christian Meisenbichler	University of Leoben, AUT
Weine Olovsson	Linköping University, SWE
Andris Gulans	Humboldt Universität zu Berlin, DEU
Dmitrii Nabok	Humboldt Universität zu Berlin, DEU
Ute Werner	Humboldt Universität zu Berlin, DEU
Giulio Biddau	Humboldt Universität zu Berlin, DEU
Pablo Garcia Risueño	Humboldt Universität zu Berlin, DEU
Stefan Kontur	Humboldt Universität zu Berlin, DEU
Hong Li	Humboldt Universität zu Berlin, DEU
Santiago Rigamonti	Humboldt Universität zu Berlin, DEU
Kathrin Glantschnig	University of Leoben, AUT

Student participants

Fatima Allouche	University of Khenchela, DZA
Danilo Neuber	EPCOS OHG, Deutschlandsberg, AUT
Sriram Poyyapakkam Ramkumar	K.U.Leuven, BEL
Jan Hermann	Faculty of Science, Charles University in Prague, CZE
Joumana Assaf	Universite de Lille 1 Sciences et Technologies, FRA
Aliakbar Ghafari	Humboldt Universität zu Berlin, DEU
Karsten Hannewald	Humboldt Universität zu Berlin, DEU
Sebastian Putz	Humboldt Universität zu Berlin, DEU
Martin Schmei	Humboldt Universität zu Berlin, DEU
Olga Turkina	Humboldt Universität zu Berlin, DEU
Christian Vorwerk	Humboldt Universität zu Berlin, DEU
Wenwu Xu	Institute of Materials Science and Technology, Friedrich-Schiller-University Jena, DEU
Myroslav Zapukhlyak	Institut für Theoretische Physik, Leibniz-Universität Hannover, DEU
Meena Devi Jeyapragasam	Institute of Mathematical Sciences, Chennai, IND
Archana Manoharan	M.Sc Materials Science, IND
Abhishek Kumar Mishra	Jawaharlal Nehru Centre for Advanced Scientific Research, IND
Luca Bursi	University of Modena and Reggio Emilia, ITA
Caterina Cocchi	Centro S3, CNR-Istituto Nanoscienze, ITA
Cristiana Di Valentin	University of Milano- Bicocca, ITA
Giovanni Garberoglio	LISC - Fondazione Bruno Kessler, ITA
Francesco Ricci	Department of Physics - University of Cagliari, ITA
Alessandro Stroppa	University of L'Aquila, ITA
Simone Taioli	Interdisciplinary Laboratory for Computational Science LISC, Trento, ITA
Yosuke Harashima	Department of Physics, Graduate School of Science, Osaka University, JPN
Juan Pablo Echeverry	Donostia International Physic Center-Basque Country University, ESP
Yunguo Li	KTH Stockholm, SWE
Baisheng Sa	KTH Stockholm, SWE
Ken-Ming Lin	Department of Physics, National Chung Cheng University, TWN
Imen Ben Amara	Faculté des sciences de Tunis-El Manar, TUN
Bahadir Altintas	Abant Izzet Baysal University, Dept. of Computer and Instructional Technologies, TUR
Danilo Puggioni	Department of Materials Science and Engineering, Drexel University, USA