Report on Workshop:

HoW exciting! Hands-on workshop on excitations in solids employing the **exciting** code

CECAM-HQ-EPFL, Lausanne, Switzerland

November 11-17, 2010

Sponsors:

CECAM, Psi-k, & SimNet Styria

Organisers:

Claudia Ambrosch-Draxl	**- University of Leoben**
Pasquale Pavone	**- Materials Center (MCL) Leoben Forschung GmbH & University of Leoben**
Clas Persson	**- Royal Institute of Technology, Stockholm**
Jürgen Spitaler	**- MCL Leoben Forschung GmbH**

Web pages:

`http://www.cecam.org/workshop-455.html`
`http://exciting-code.org/how-exciting`

Summary

The CECAM workshop was devoted to the presentation of both basic concepts and computational tools (embedded in the software package **exciting**) which are needed for the calculations of various excitations in solids. The workshop took place at the CECAM Head Quarter in Lausanne, Switzerland, in November 2010. It turned out to be very successful and reached all the expected goals. The participants enjoyed a varied programme of interesting lectures and discussions.

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 and lattice vibrations 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 (Ambrosch-Draxl, Meisenbichler Spitaler, Pavone, Sagmeister) 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 (Rubio), many-body perturbation theory (Reining), phonons and electron-phonon coupling (Baroni), superconductivity (Gross), magnetism (Nordström), large scale simulations (Blaha, Gonze), thermodynamic and mechanical properties (Neugebauer), and multi-scale modelling based on ab-initio approaches (Scheffler). A special talk was also organized to address the future evolution in terms of memory and speed of computing in condensed matter physics (Schulthess).

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 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`. The list and description of the tutorial exercises is also available at `http://exciting-code.org/cecam-exercises`.

There were a total of 47 scientific participants, among them 4 organisers, 11 lecturers, 6 tutors, and 26 student participants from institutions of 13 countries, including various European nations, Mexico, Japan, and 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 - November 11, 2010

08:40 - 09:00	Welcome
09:00 - 10:00	**Kieron Burke** *ABC of DFT*
10:00 - 10:30	**Claudia Ambrosch-Draxl** *APW-derived basis sets*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *Electronic structure*
12:45 - 14:00	Lunch Break
14:00 - 14:30	**Christian Meisenbichler** *Exciting installations and user tools*
14:30 - 16:00	Exercises: *I/O and templates*
16:00 - 16:30	Coffee Break
16:30 - 17:30	Exercises: *I/O and templates*
17:30 - 18:30	**Thomas Schulthess** *Petascale computing in condensed matter physics*

Day 2 - November 12, 2010

09:00 - 10:00	**Kieron Burke** *EFG of DFT*
10:00 - 11:00	Exercises: *DFT*
11:00 - 11:15	Coffee Break
11:15 - 12:00	Exercises: *User projects*
12:00 - 13:30	Lunch Break
13:30 - 14:30	**Jörg Neugebauer** *Ab-initio thermodynamics:* *From excitations to material properties*
14:30 - 15:00	**Jörg Neugebauer** *Introduction to cluster expansion*
15:00 - 15:30	**Jürgen Spitaler** *ATAT@exciting*
15:30 - 16:00	Coffee Break
16:00 - 18:00	Exercises: *Cluster expansion*

Day 3 - November 13, 2010

09:00 - 10:00	**Stefano Baroni** *Lattice excitations*
10:00 - 10:45	**Pasquale Pavone** *Stress and strain in exciting*
11:00 - 11:15	Coffee Break
11:15 - 12:45	Exercises: *Elastic constants*
12:45 - 14:00	Lunch Break
14:00 - 14:30	**Pasquale Pavone** *Forces, phonons, and thermal properties in exciting*
14:30 - 16:15	Exercises: *Structure optimization and phonons*
16:15 - 16:45	Coffee Break
16:45 - 18:15	Exercises: *Energy functionals*

Day 4 - November 14, 2010

Excursion

Day 5 - November 15, 2010

09:00 - 10:00	**Angel Rubio** *Time-dependent DFT*
10:00 - 10:30	**Stephan Sagmeister** *TDDFT in exciting*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *Linear-response TDDFT*
12:45 - 14:00	Lunch Break
14:00 - 15:00	**Lucia Reining** *Many-body perturbation theory:* *From fundamental ideas to use in practice*
15:00 - 15:30	**Stephan Sagmeister** *BSE in exciting*
15:30 - 16:00	Coffee Break
16:00 - 18:00	Exercises: *Excitonic effects via BSE*

Day 6 - November 16, 2010

09:00 - 10:00	**Lars Nordström** *Exciting behaviour of exotic magnetic materials: Up and down and around*
10:00 - 10:30	**Jürgen Spitaler** *Magnetism in exciting*
10:30 - 10:45	Coffee Break
10:45 - 12:45	Exercises: *Magnetism*
12:45 - 14:00	Lunch Break
14:00 - 15:00	**Xavier Gonze** *Addressing large-scale software development and maintenance from a physicist point of view*
15:00 - 16:00	**Peter Blaha** *Challenges of large scale simulations with all-electron methods*
16:00 - 16:30	**Claudia Ambrosch-Draxl** *Core-level spectroscopy: Core electrons and relativistic effects*
16:30 - 16:45	Coffee Break
16:45 - 18:45	Exercises: *Core excitations via BSE*

Day 7 - November 17, 2010

09:00 - 10:00	**E.K.U. Gross** *Superconductivity*
10:00 - 11:45	Exercises: *Advanced user projects*
11:45 - 12:00	Coffee Break
12:00 - 13:00	**Matthias Scheffler** *Multi-scale modeling of the function of materials from first principles*

List of participants

Organisers

Claudia Ambrosch-Draxl	University of Leoben, AUT
Pasquale Pavone	MCL Leoben & University of Leoben, AUT
Clas Persson	Royal Institute of Technology, Stockholm, SWE
Jürgen Spitaler	MCL Leoben, AUT

Lecturers

Stefano Baroni	International School for Advanced Studies, Trieste, ITA
Peter Blaha	Technical University of Vienna, AUT
Kieron Burke	University of California Irvine, USA
Xavier Gonze	Universite Catholique de Louvain, BEL
E.K.U. Gross	Max Planck Institute of Microstructure Physics, Halle, DEU
Jörg Neugebauer	Max-Planck Institute for Iron Research, Düsseldorf, DEU
Lars Nordström	University of Uppsala, SWE
Lucia Reining	Ecole Polytechnique, Palaiseau, FRA
Angel Rubio	Universidad del País Vasco, San Sebastian, ESP
Matthias Scheffler	Fritz-Haber-Institut der MPG, Berlin, DEU
Thomas Schulthess	Swiss National Supercomputer Center, Zürich, CHE

Tutors

Thomas Dengg	University of Leoben, AUT
Rostam Golesorkhtabar	MCL Leoben & University of Leoben, AUT
Dominik Legut	MCL Leoben & University of Leoben, AUT
Christian Meisenbichler	University of Leoben, AUT
Weine Olovsson	University of Leoben, AUT
Stephan Sagmeister	MCL Leoben & University of Leoben, AUT

Student participants

Audrius Alkauskas	Ecole Polytechnique Fédérale de Lausanne, CHE
Gustavo Baldissera	Royal Institute of Technology, Stockholm, SWE
Alexander Baral	University of Kaiserslautern, DEU
Jordan Bieder	CEA, FRA
Javier Camarillo Cisneros	Centro de Investigacion en Materiales Avanzados, MEX
Rongzhen Chen	Royal Institute of Technology, Stockholm, SWE
Maofeng Dou	Royal Institute of Technology, Stockholm, SWE
David Egger	Graz University of Technology, AUT
Tamas Hornos	University of Oslo, NOR
Kerstin Hummer	University of Vienna, AUT
Hidekazu Ikeno	Kyoto University, JAP
Steffen Kaltenborn	University of Kaiserslautern, DEU
Deniz Kecik	Paul Scherrer Institut, Villigen, CHE
Martin Krobath	Materials Center Leoben Forschung GmbH, AUT
Shen Li	Royal Institute of Technology, Stockholm, SWE
Daniel Lueftner	Materials Center Leoben Forschung GmbH, AUT
Mohammad Reza Monazam	Johannes Kepler University, Linz, AUT
Dmitrii Nabok	University of Leoben, AUT
Markus Orthaber	Materials Center Leoben Forschung GmbH, AUT
Ferdinand Rissner	Graz University of Technology, AUT
Oleksandr Romanyuk	Institute of Physics, ASCR, Prague, CZE
Iván Santos	University of Valladolid, ESP
Simon Schneider	Ecole Polytechnique Fdrale de Lausanne, CHE
Cosima Schuster	Universität Augsburg, DEU
Svenja Vollmar	University of Kaiserslautern, DEU
Hanyue Zhao	Royal Institute of Technology, Stockholm, SWE