Report of the CAMD Summer School 2012 on the

Electronic Structure Theory
&
Materials Design

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In brief:

The Psi-k sponsored “CAMD Summer School 2012 Electronic Structure Theory and Materials Design” was held in the week August 11-17, 2012 at the Technical University of Denmark in Lyngby. Thanks to the 67 external attentive summer school students and the 15 very helpful invited lecturers the school was the nice success that we had hoped for.

Motivation:

The motivation for the school was that the era of cheap fossil fuels over the next few decades is expected to come to an end. Arguably making the development of sustainable energy solutions the most important scientific and technical challenge of our time. In order to address these and other technical challenges, we must in the future present a significantly improved capability to rationally design new materials. Computational design of new materials has been demonstrated in a few test cases, but in order to carry out systematic computational design of new materials for e.g. energy storage, fuel synthesis, and light harvesting, a number of methodological improvements are needed. Methods dealing with the description of electron transfer processes at surfaces in solid or liquid electrolytes, for photo-absorption and charge separation in extended solids, and for electronic localization in insulators have to be improved. Developing better handles on the errors in the electronic structure description (e.g. through Bayesian Error Estimation methods) may also prove critical. In order to begin addressing these challenges, the summer school focused on the fundamental concepts and the current status of the areas of DFT, and DFT implementations, TDDFT, excited states, thermodynamic properties derived from electronic structure calculations, modern xc-functionals, properties of surfaces and electron transfer at these, energy materials, error estimation, catalysis, electro-catalysis, and materials design strategies.

Purpose:

The summer school aimed to teach the students how electronic structure theory can be used for materials design. An introduction to density functional theory with particular emphasis on practical methodology and implementation aspects was given and extensions beyond the standard DFT formalism were discussed. A significant focus was on the methodology applied “on-top” of electronic structure calculations to enable the search after new functional materials.

The summer school was a combination of lectures given by experts in the field and exercises giving hands-on-experience with the Atomic Simulation Environment (ASE) supervised by expert users. The ASE is a general purpose open source simulation environment that can be used to setup, control, and analyze electronic structure simulations carried out in a variety of electronic structure codes, e.g. including GPAW, Dacapo, VASP, Octopus, AbInit, ASAP, Siesta, and others.

Subjects:

The subjects covered in lectures were more specifically:

- The fundamentals of Density Functional Theory
- Strategies for solving the Kohn-Sham equations
- Projector Augmented Wave Implementation
- Exchange-correlation functionals
- Error estimation in Density Functional Theory
- Time-dependent DFT
- Many-body approaches to the electronic structure problem
- Quantum electron transport theory
- Thermodynamic properties and kinetics from DFT
- Energy Materials
- Chemistry at surfaces/Heterogeneous Catalysis
- Electrochemistry
- Materials Informatics

Lecturers:

The Invited Lecturers were:

- Kieron Burke, University of California Irvine, USA
- Jussi Enkovaara, CSC - IT Center for Science, Finland
- Georg Kresse, University of Vienna, Austria
- Angel Rubio, Universidad del Pais Vasco, Spain
- Hannes Jonsson, University of Iceland, Iceland
- Bjørk Hammer, University of Aarhus, Denmark
- Suljo Linic, University of Michigan, USA
- Jens K. Nørskov, Stanford University, USA
- Per Siegbahn, University of Stockholm, Sweden
- Troy Van Voorhis, MIT, USA
- Mike Finnis, Imperial College London, UK
- Per Hyldgaard, Chalmers University of Technology, Sweden
- Anubhav Jain, Lawrence Berkeley National Laboratory, USA
- Hardy Gross, Freie Universität Berlin, Germany
- Thomas Bligaard, SLAC National Accelerator Laboratory, USA

who gave presentations on their respective fields of expertise. In addition talks were presented by the local scientific organizing committee.

Venue:

The CAMD summer school was held at the Technical University of Denmark in the pleasant Lyngby area North of Copenhagen.

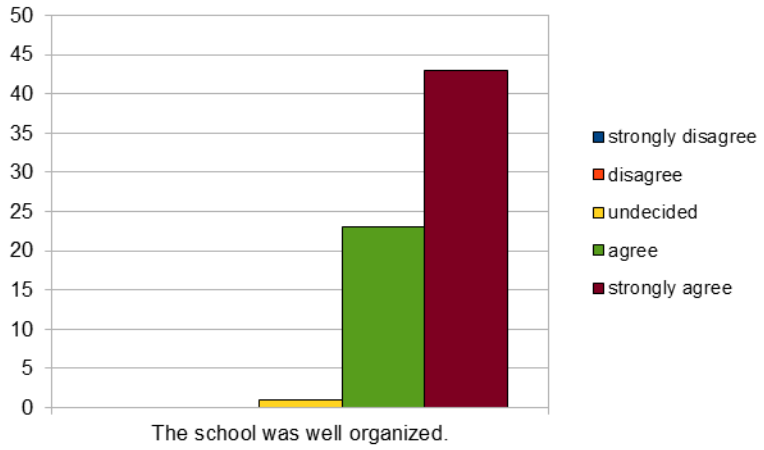
Credits:

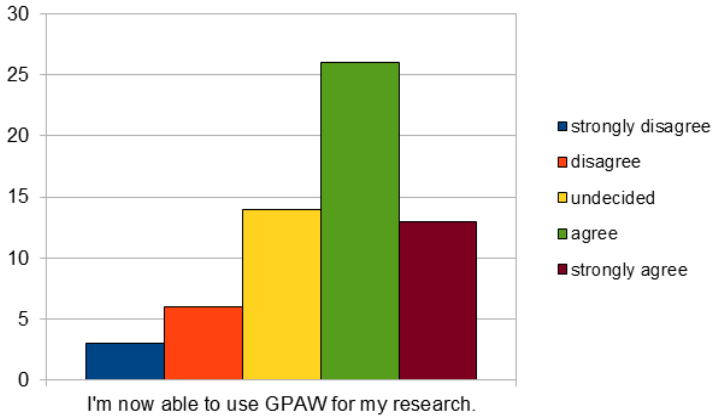
A diploma which certified that the students had participated and earned 2.5 ECTS points was issued to the participants upon their completion of the summer school.

The participants and their evaluation:

The participants were primarily PhD-students (more than 75) but there were also a few post docs and professors. Most had a background in physics, but there were also some chemists and some with a background in Chemical engineering and materials science. More than 40 of the participants were DFT users.

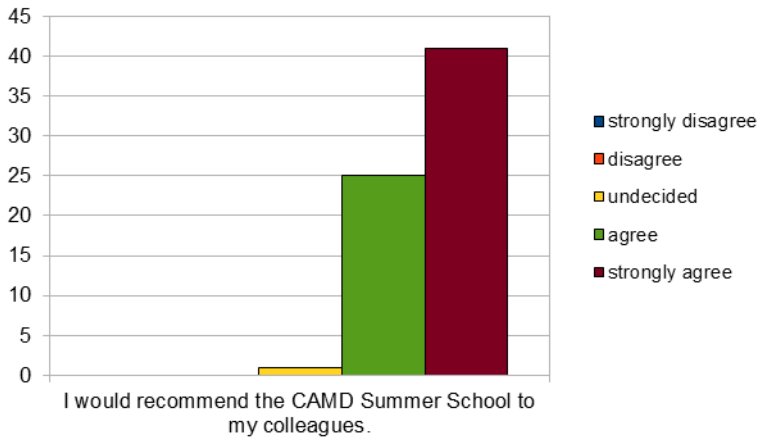
After the termination of the summer school, the participants were asked to evaluate a number of criteria, and generally we were quite happy with the outcome of the evaluation. In the figures we depict some of the responses of the students.





The students seemed to find that the administrational organization of the school was quite satisfactory, and somewhat to the surprise of the organizers, many of the summer school students, who did not know the electronic structure code GPAW before the school, actually learned it so well, that they now feel that they can use it directly in their research.

We were very happy that a good fraction of the participants would recommend another CAMD Summer School to their colleagues.



The CAMD Summer School
Electronic Structure Theory and Materials Design
August 11-17, 2012
(Supported by the Psi-k Network and CECAM)

Programme:

Saturday, August 11, 2012:

14:00-19:00 Arrival to the guest houses on the DTU campus – keys have to be picked up at Building 311
19:00- Welcome reception (Chinese dinner) at DTU, Building 311, 1. floor

Sunday, August 12:

08:30-09:15 Breakfast
09:15-09:30 Welcome (Karsten W. Jacobsen)
09:30-10:30 Fundamentals of DFT 1 (Kieron Burke)
10:30-11:00 Coffee
11:00-12:00 Fundamentals of DFT 2 (Kieron Burke)
12:00-14:00 Lunch
14:00-15:00 Projector augmented wave method and the GPAW code (Jussi Enkovaara)
15:00-15:30 Coffee
15:30-16:30 The Atomic Simulation Environment and introduction to the databar (Jakob Schiøtz)
16:30-18:00 Setting up for computer exercises

Monday, August 13:

08:30-09:30 Breakfast
09:30-10:30 Total energies from many-body perturbation theory (Georg Kresse)
10:30-11:00 Coffee
11:00-12:00 Excited states from many-body perturbation theory (Georg Kresse)
12:00-13:30 Lunch
13:30-14:15 Spectroscopy from time-dependent DFT (Angel Rubio)
14:15-15:15 Coffee
15:15-16:00 Real time dynamics with TDDFT (Angel Rubio)
16:00-18:00 Computer exercises
18:00-20:00 Poster session (supported by QuantumWise A/S)

Tuesday, August 14:

08:30-09:30 Breakfast
09:30-10:30 Path techniques and reaction rates (Hannes Jonsson)
10:30-11:00 Coffee
11:00-12:00 Adsorbate-surface interactions (Bjørk Hammer)
12:00-13:30 Lunch
13:30-14:30 Catalysis from DFT (Suljo Linic)
14:30-15:00 Coffee
15:00-15:45 Concepts and trends in surface reactivity (Jens Nørskov)
15:45-16:00 Short break with coffee
16:00-16:45 Concepts and trends in surface reactivity (Jens Nørskov)
16:45-18:30 Computer exercises

Wednesday, August 15:
08:00-09:00 Breakfast
09:00-10:00 Structure and function of enzymes (Per Siegbahn)
10:00-10:30 Coffee
10:30-11:30 Electron transfer dynamics in solution (Troy Van Voorhis)
11:30-11:45 Short break
11:45-12.30 Exchange-correlation functionals with error bars (Karsten W. Jacobsen)
12:30-13:30 Lunch
13:30-15:00 Computer exercises
Rest of the day: Excursion and social dinner

Thursday, August 16:
08:30-09:30 Breakfast
09:30-10:30 Interfaces and defects (Mike Finnis)
10:30-11:00 Coffee
11:00-12:00 Non-adiabatic processes at surfaces (Jakob Schiøtz)
12:00-13:30 Lunch
13:30-14:30 Materials informatics (Anubhav Jain)
14:30-15:00 Coffee
15:00-15:45 Van der Waals interactions (Per Hyldgaard)
15:45-16:00 Small break with coffee
16:00-16:45 Density Matrix Functional Theory (Hardy Gross)
16:45-18:30 Computer exercises

Friday, August 17:
08:30-09:30 Breakfast
09:30-10:30 Electrochemistry with DFT (Jan Rossmeisl)
10:30-11:00 Coffee
11:00-12:00 Quantum electron transport (Kristian Thygesen)
12:00-13:30 Lunch
13:30-14:30 Catalysis informatics (Thomas Bligaard)
14:30-15:00 Coffee
15:00-15:45 Energy Materials (Tejs Vegge)
15:45-16:00 Closing remarks (Karsten W. Jacobsen)

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