Report of the CAMD Summer School 2014 on the

Electronic Structure Theory and Materials Design

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In brief

The Psi-k sponsored "CAMD Summer School 2014 Electronic Structure Theory and Materials Design" was held in the week August 17-22, 2014 at the Technical University of Denmark in Lyngby. Thanks to the more than 80 external attentive summer school students and the 11 very helpful invited lecturers the school was the nice success that we had hoped for.

Motivation

Our current wealth is largely based on the access to cheap fossil fuels. This era is coming to an end, arguably making the development of sustainable energy solutions the most important scientific/technical challenge of our time. Catalysis will be central in addressing this challenge, and in converting the essentially unlimited influx of energy from the sun into useful chemically stored fuels through catalytic, electrocatalytic, and photocatalytic processes. Computational design of solid (photo)catalysts have been demonstrated in a few test cases, but in order to carry out systematic computational design of electrocatalysts and photocatalysts, the methodology has to be established for describing 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. Developing improved handles on the errors in the electronic structure description (e.g. through Bayesian Error Estimation) may also prove critical. In order to start addressing these challenges, we will teach the fundamental concepts and the current status of the areas of basic DFT, and DFT implementations, TDDFT, excited states, thermodynamic properties derived from electronic structure calculations, modern exchange-correlation functionals, properties of surfaces and electron transfer at these, energy materials, error estimation, catalysis, electrocatalysis 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:

- Nicola Marzari, EPFL, Switzerland
- Georg Kresse, University of Vienna, Austria
- Hardy Gross, Freie Universität Berlin, Germany
- Alexandre Tkatchenko, Fritz Haber Institute, Germany
- Hannes Jonsson, University of Iceland
- Bjørk Hammer, University of Aarhus, Denmark
- Jens K. Nørskov, Stanford University, USA
- Joost VandeVondele, ETH Zürich, Switzerland
- Martti Puska, Aalto University, Finland
- Stefano Curtarolo, Duke University, USA
- 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.

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 figure 1 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 were satisfied with the topics covered. Many of the summer school students, the majority of whom 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.

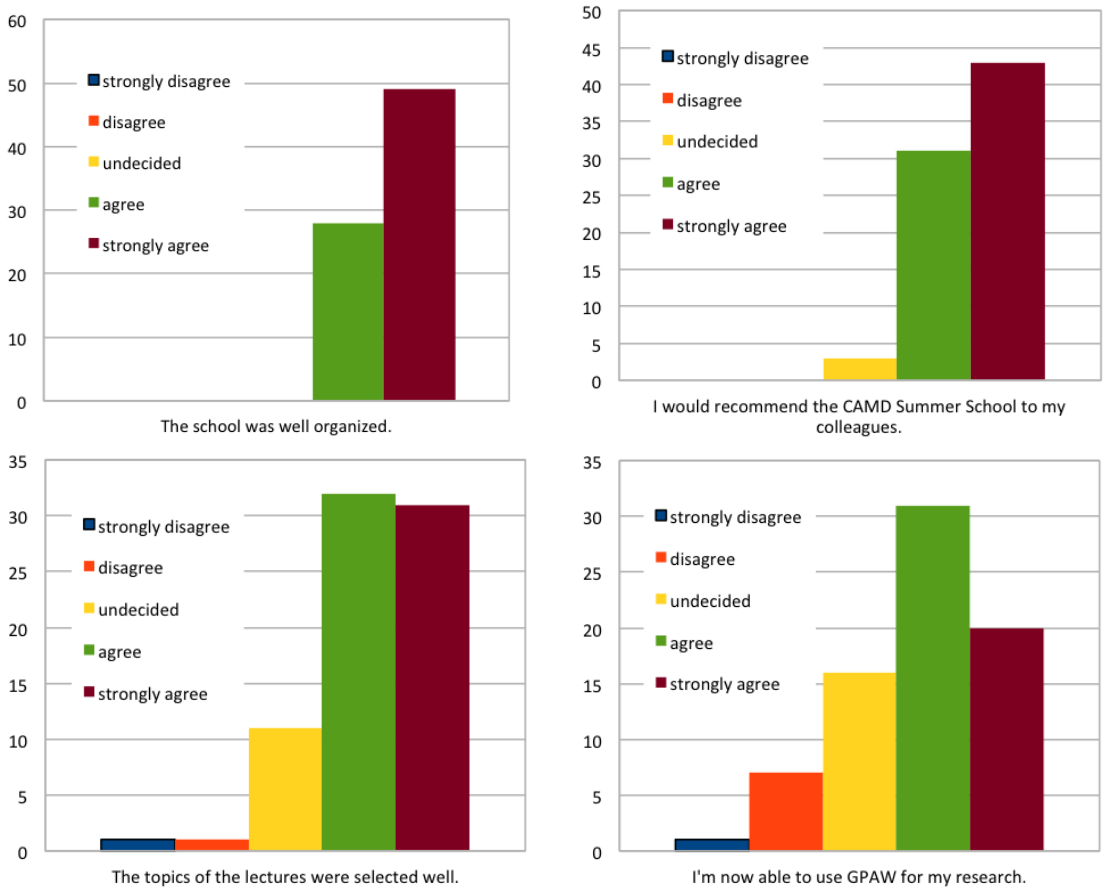

Figure 1: The main results of the evaluation by the participants.

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

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