Report of the CAMD Summer School 2010 on the

Electronic Structure theory
&
Materials Design

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In brief:

The Psi-k sponsored "CAMD Summer School 2010 Electronic Structure Theory and Materials Design" was held in the week August 14-20, 2010 at the Technical University of Denmark in Lyngby. Thanks to the 70 attentive summer school students and the 12 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 beyond GGA
- Error estimation in Density Functional Theory
- Time-dependent DFT
- Many-body approaches to the electronic structure problem
- Van der Waals descriptions
- Superconductivity with DFT
- Quantum electron transport theory
- Spectroscopy from DFT
- Thermodynamic properties and kinetics from DFT
- Energy Materials
- Chemistry at surfaces/Heterogeneous Catalysis
- Electrochemistry
- Materials Informatics

Lecturers:

The Invited Lecturers were:
Peter Blöchl, TU Clausthal
Kieron Burke, UC Irvine
Mike J. Gillan, UC London
E.K.U. Gross, Freie Universität Berlin
Martin Head-Gordon, UC Berkeley
Hannes Jónsson, University of Iceland
John Kitchin, Carnegie Mellon University
Bengt Lundqvist, Chalmers Technical University
Manos Mavrikakis, UW Madison
Lucia Reining, École Polytechnique
Lars G. M. Pettersson, Stockholm University
Jens K. Nørskov, Stanford University
who gave presentations on their respective fields of expertise. In addition talks were presented by the local scientific organizing committee.
Venue:

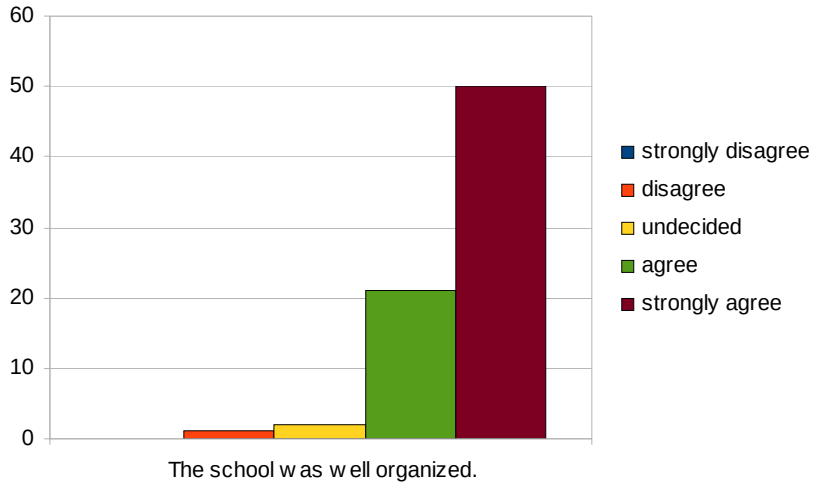
Credits:

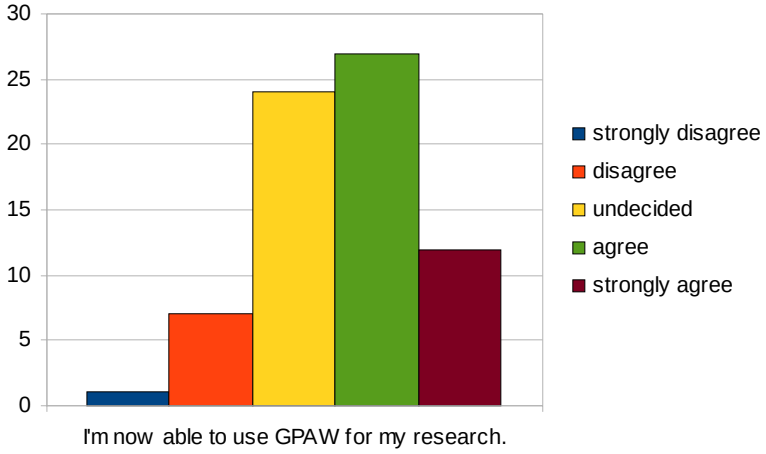
A diploma which certified that the students had participated and earned 2.5 ECTS points was issued to the participants upon their completion of the summer school.

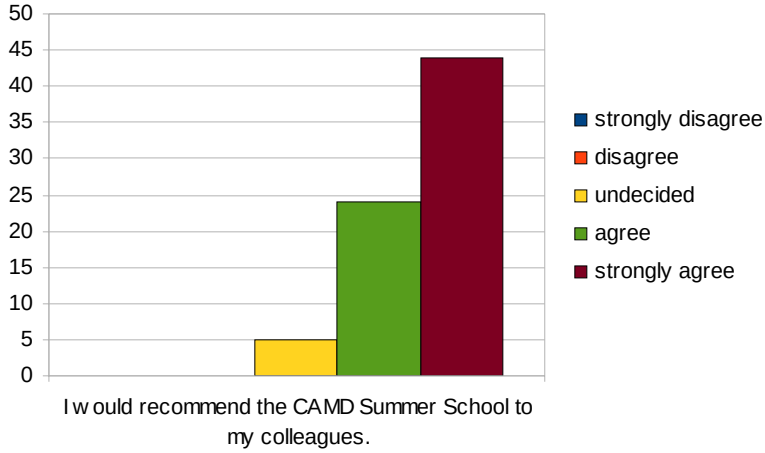
The participants and their evaluation:

The participants were primarily PhD-students (more than 60) but there was also a few post docs. Most had a background in physics (44), but there were also some chemists (23) and some with a background in Chemical engineering and materials science. More than 50 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.







Final Program

The 2010 CAMD Summer School
on
Electronic Structure Theory and Materials Design
(Supported by the Psi-k Network)

August 14-20, 2010

Saturday, August 14, 2010:

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 15, 2010:

08:45-09:30	Breakfast
09:30-10:45	Fundamentals of DFT 1 (Kieron Burke)
10:45-11:15	Coffee break
11:15-12:30	Fundamentals of DFT 2 (Kieron Burke)
12:30-14:00	Lunch
14:00-15:00	Path techniques and reaction rates in DFT (Hannes Jónsson)
15:00-15:30	Coffee break
15:30-16:30	Van der Waals in DFT (Bengt Lundqvist)
16:30-16:45	Short break (with coffee)
16:45-17:15	Description of the data bar system (Jens Jørgen Mortensen)
17:15-18:30	Getting set to go in the data bar, etc. (Jens Jørgen + The entire team)

Monday, August 16, 2010:

08:45-09:30	Breakfast
09:30-10:30	Strategies for solving the Kohn-Sham equations (Peter Blöchl)
10:30-11:00	Coffee
11:00-12:00	Projector Augmented Wave Implementation (Peter Blöchl)
12:00-13:30	Lunch
13:30-14:15	Adsorbate-surface interactions (Jens Nørskov)
14:15-14:30	Short break (with coffee)
14:30-15:15	Concepts and trends in surface reactivity (Jens Nørskov)
15:15-18:00	Exercises (ASE/GPAW)
18:00-20:00	Poster session and refreshments

Tuesday, August 17, 2010:

08:45-09:30	Breakfast
09:30-10:15	Exchange-correlation functionals beyond GGA (Martin Head-Gordon)
10:15-10:30	Short break (with coffee)
10:30-11:15	Excited states in extended systems (Martin Head-Gordon)
11:15-11:45	Coffee break
11:45-12:30	Error estimation in DFT (Karsten Jacobsen)
12:30-14:00	Lunch
14:00-14:45	Catalysis from DFT (Manos Mavrikakis)
14:45-15:15	Coffee break
15:15-16:00	Adsorbate-adsorbate interactions (John Kitchin)
16:00-16:30	Presentation of the CAMD Linux-cluster technology (Ole H. Nielsen)
16:30-18:30	Exercises (GPAW)+Tour to computer room for those who are interested (OHN)

Wednesday, August 18, 2010:

08:45-09:30 Breakfast
09:30-10:15 Time Dependent DFT (Hardy Gross)
10:15-10:30 Short break (with coffee)
10:30-11:15 Superconductivity in DFT (Hardy Gross)
11:15-11:45 Coffee break
11:45-12:30 Quantum electron transport (Kristian Thygesen)
12:30-13:30 Lunch
13:30-15:00 Exercises (GPAW)
15:15- Departure by bus from Building 311 –
Excursion to the Planetarium in Copenhagen followed by dinner at Brasserie Nimb, Tivoli. After dinner you can visit Tivoli on your own as you like

Thursday, August 19, 2010:

08:45-09:30 Breakfast
09:30-10:30 Spectroscopy from DFT (Lars G.M. Pettersson)
10:30-11:00 Coffee break
11:00-12:00 Many-body approaches (Lucia Reining)
12:00-13:30 Lunch
13:30-14:15 Electro-catalytic reactions (Jan Rossmeisl)
(* 14:15-19:00 ASE/GPAW install session on personal laptops (Marcin + Jens Jørgen) *)
14:15-18:00 Exercises (GPAW)
- Afternoon coffee and cake will be available in Building 311

Friday, August 20, 2010:

Check out and handing in keys to your rooms to Marianne before 09:30.

08:45-09:30 Breakfast
09:30-10:15 Thermodynamic Properties from DFT 1 (Mike J. Gillan)
10:15-10:30 Short break (with coffee)
10:30-11:15 Thermodynamic Properties from DFT 2 (Mike J. Gillan)
11:15-11:45 Coffee break
11:45-12:30 Energy materials (Tejs Vegge)
12:30-14:00 Lunch
14:00-14:45 Catalysis Informatics (Thomas Bligaard)
14:45-15:00 Closing remarks (Karsten Jacobsen)
15:00-16:00 Afternoon cake and diffusion
16:00 Summer School closed - departure

(Last updated on August 10, 2010)

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