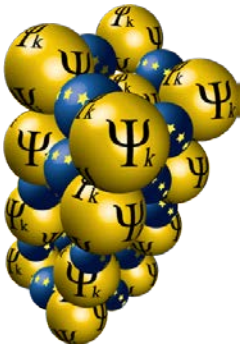

Report of the CAMD Summer School 2018 on the

Electronic Structure Theory
&
Materials Design

Scientific Organizers:

Karsten W. Jacobsen, Department of Physics, DTU
Kristian S. Thygesen, Department of Physics, DTU
Jakob Schiøtz, Department of Physics, DTU
Thomas Olsen, Department of Physics, DTU
Tejs Vegge, Department of Energy Conversion and Storage, DTU

Administrative Organizer:

Marianne Ærsøe, Department of Physics, DTU

In brief:

The Psi-k sponsored “CAMD Summer School 2018 Electronic Structure Theory and Materials Design” took place in the week August 12-17, 2018 at Strandhotel Marienlyst in Helsingør, Denmark. Thanks to the more than 100 external attentive summer school students and the 15 very helpful invited lecturers, the school was the nice success that we had hoped for. The school taught PhD students from all over the world the basic and more advanced concepts in modern electronic structure theory including ground state density functional theory (DFT), many-body methods materials informatics and machine learning. Emphasis was put on the methodology applied “on-top” of ab-initio calculations which is essential for the computational design of new functional materials.

Scientific summary:

The primary purpose of this summer school was to teach the students how electronic structure theory can be used for materials design. An introduction to density functional theory (DFT) with particular emphasis on practical methodology and implementation aspects was given. Extensions beyond the standard DFT formalism including time-dependent DFT, spin-orbit coupling, Berry phases, and Many-body perturbation theory were discussed. In addition, a full day was devoted to machine learning and materials informatics. The subjects provided the students with a basic toolbox that will allow them to perform first principles analysis of a large variety of problems in physics and chemistry. For example, quasiparticle excitations in the GW approximation, excitons from the Bethe-Salpeter Equation (BSE), time-dependent density functional theory (TDDFT), correlation energies from the random phase approximation, Berry phases and topological insulators, heterogeneous catalysis and electrochemistry. The students were then taught how to embed electronic structure calculations in a framework that facilitates design of materials with specific properties.

The summer school consisted of lectures by international experts in the field followed by computer exercises giving hands-on-experience with the concepts discussed in the lectures. The computer exercises were based on the electronic structure code GPAW and the Atomic Simulation Environment (ASE). GPAW is based on the projector-augmented wave methodology and can perform computations on real space grids, plane waves or localized atomic orbitals. Besides ground state DFT, GPAW can perform various post-DFT electronic structures calculations such as GW, BSE, and TDDFT – all exemplified by pedagogical exercises. 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 VASP, Octopus, GPAW, Dacapo, AbInit, ASAP, and Siesta. The exercises were supervised by expert users of ASE and GPAW.

During the exercises, the students worked in small groups with the focus on learning to produce publication quality simulations on a small computer-

cluster. All students had to do one introductory exercise, which served to introduce the students to python and ASE. After completing this, the students could choose between five specialized tutorials on photovoltaics, machine learning, magnetism, catalysis or batteries that were all designed specifically for the students at the school.

Invited lecturers and subjects covered:

- Hardy Gross, Max Planck Institute of Microstructure Physics, Germany
  "Fundamentals of DFT and TDDFT"

- Jens Nørskov, Stanford University, USA
  "Computational Design in Catalysis"

- Hannes Jonsson, University of Iceland
  "Rate Theory"

- Bjørk Hammer, Aarhus University, Denmark
  "Structures and Reactions at Surfaces" and "Machine Learning and Structural Search"

- Jan Rossmeisl, University of Copenhagen, Denmark
  "Electrochemistry"

- Georg Kresse, University of Vienna, Austria
  "Many-Body Perturbation Theory"

- Claudia Draxl, Humboldt-Universität Berlin, Germany
  "Theoretical Spectroscopy"

- Nicola Marzari, EPFL, Switzerland
  "2D materials"

- Christopher Wolverton, Northwestern University, USA
  "Machine Learning and Materials Science"

- Anatole von Lilienfeld, University of Basel, Switzerland
  "Machine Learning and Chemistry"

- Thomas Bligaard, SLAC National Accelerator Laboratory, USA
  "Materials Informatics"

- Yan Sun, Max-Planck-Gesellschaft, Germany
  "Topological States of Matter"

- Stefano Curtarolo, Duke University, USA
  "Discovery of Novel Electronic Materials"

- Aron Walsh, Imperial College London, UK
  "Materials Modelling for Solar Cells: Perovskites and Beyond"

- Kieron Burke, University of California, USA
  "The Future of DFT"

Lecturers by organizers and subjects covered:

- Jakob Schiøtz, DTU
  "Electronic structure tools: ASE and GPAW"

- Kristian S. Thygesen, DTU
  "Excitations in 2D materials"

- Karsten W. Jacobsen, DTU
  "Machine Learning Basics"

- Thomas Olsen, DTU
  "Spin-orbit physics"

- Tejs Vegge, DTU
  "Batteries"

Venue:

The CAMD summer school was held at Marienlyst Strandhotel in Helsingør in the beautiful North Zealand.

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 international PhD-students but there were also quite a few post docs and other students. The participants' background was in physics, chemistry, 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 the figures we depict some of the responses of the students. The students seemed to find that the overall scientific and academical organization of the school was quite satisfactory.

	☹	😕	😐	🙂	😀
The information received before arriving was sufficient.	0	0	2	19	58
The school was well organized.	0	0	1	13	65
The lectures satisfied my expectations.	1	1	9	34	34
The exercises satisfied my expectations.	2	3	16	36	22
I would recommend the CAMD Summer School to my colleagues.	0	0	5	20	54

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

Before the summer school a lot of work was put into making the exercises more structured this year. The participants could choose between 5 subjects for the exercises:

- Batteries
- Catalysis
- Machine Learning
- Magnetism
- Photovoltaics

	☹	😕	😐	🙂	😀
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	☹	😕	😐	🙂	😃
The level of the lectures was adequate to my knowledge.	3	2	12	29	33
The number of lectures per day was adequate.	1	0	3	20	55
The topics of the lectures were selected well.	0	2	5	19	53
The plenary room was suitable.	0	1	2	11	65

Since this was the first time the summer school was taking place outside of DTU, we were also very pleased to see, that the participants liked the venue.

	☹	😕	😐	🙂	😃
The accommodation was adequate	0	0	0	6	73
The meals were adequate	2	2	4	7	64
I used the spa facilities	8	0	6	3	62

Name	Name of University/Institution/Company	Country
Aayush Singh	Stanford University	United States
Agnieszka Jamróz	Faculty of Pysics, University of Warsaw	Poland
Aleksei Ivanov	University of Iceland	Iceland
Alessia Di Vito	Università degli Studi di Roma Tor Vergata	Italy
Alexander Genest	Institute of High Performance Computing, A*STAR	Singapore
Alexander Tygesen	Technical University of Denmark	Denmark
Alvaro Posada Borbón	Chalmers University of Technology	Sweden
Amanda Petersen	University of Copenhagen	Denmark
Amin Mirzai	Lund university	Sweden
Ananth Govind Rajan	Massachusetts Institute of Technology	United States
Anders Riis-Jensen	Technical University of Denmark	Denmark
Anjli Patel	Stanford University	United States
Ankit Jain	DTU	United States
Antti Pihlajamäki	University of Jyväskylä	Finland
Arghya Bhowmik	DTU Energy	Denmark
Armin Salmasi	KTH royal institute of technology	Sweden
Artem Samtsevych	Skolkovo Institute of Science and Technology	Russia
Asbjørn Rasmussen	DTU	Denmark
August Edwards Guldberg Mikkelsen	DTU	Denmark
Axel Forslund	KTH Royal Institute of Technology	Sweden
Caitlin Casey-Stevens	University of Otago	New Zealand
Charlie Ruffman	University of Otago	New Zealand
Charlotte Kirk	Stanford University	United States
Christian Søndergaard Pedersen	Danmarks Tekniske Universitet	Denmark
Daniele Torelli	DTU	Denmark
David Codony	Universitat Politècncica de Catalunya	Spain
Davide Gambino	Department of Physics, Chemistry and Biology (IFM), Linköping University	Sweden
Delwin Perera	Technische Universität Darmstadt	Germany
Deniz Yildiz	Villanova University	United States
Dmitry Gulevich	ITMO University	Russia
El-Abed Haidar	The University of Sydney	Australia
Emile Durant	University of Liverpool	United Kingdom
Esko Makkonen	Aalto University	Finland
Estefania Garijo Del Rio	Technical University of Denmark	Denmark
Fan Wang	Leibniz Institute for Catalysis. V.	Germany
Felix Lochner	Max-Planck-Institut für Eisenforschung	Germany
Félix Musil	EPFL - IMX - COSMO	Switzerland
Geoffrey Weal	University of Otago	New Zealand
Hao Wan	University of Copenhagen	Denmark
Hassan Aljama	Stanford University	United States
Hassan Ouhbi	Department of Chemistry and Biochemistry, University Of Bern	Switzerland
Heine Anton Hansen	DTU Energy	Denmark
Henrik Lund Mortensen	Aarhus University, IFA	Denmark
Herbert Mączko	Wroclaw University of Science and Technology	Poland
Hongbiao Tao	University of Alberta	Canada
Ivano Eligio Castelli	DTU Energy	Denmark
Jack Pedersen	University of Copenhagen	Denmark
Jaclyn Lunger	Massachusetts Institute of Technology	United States
Jacob Wilson	Imperial College Lodnon	United Kingdom
Jamoliddin Khanifaev	Max-Planck Institute for Iron research	Germany
Jens Kildgaard	DTU Energy	Denmark
Jingjing Shao	Freie University Berlin	Germany
Jodie Yuwono	Monash University	Australia
Johan Tidholm	Linköping University	Sweden
Jorge Diogo Marques Laranjeira	CICECO-Aveiro Institute of Materials	Portugal
Jose Antonio Garrido Torres	Stanford University	United States
Joseph Gauthier	Stanford University	United States
Juan Maria García Lastra	DTU Energy	Denmark
Juan Santiago Cingolani	Technische Universität München	Germany
Justin Villard	Ecole Polytechnique Fédérale de Lausanne	Switzerland
Kai Sellschopp	Hamburg University of Technology	Germany
Kangli Wang	Free University of Berlin	Germany
Karun Kumar Rao	University of Houston	United States
Katrine Svane	Technical University of Denmark	Denmark
Kirsten Winther	SLAC National Accelerator Laboratory	United States

Name	Name of University/Institution/Company	Country
Kris Brown	Stanford University	United States
Lauren Walters	Northwestern Univ	United States
Leila Ben Mahfoud	Laboratoire Hubert Curien, Université Jean-Monnet, Saint-Etienne	France
Lev Martinez Aguilera	Technical University of Denmark	Denmark
Lin Chen	Chalmers University of Technology	Sweden
Luca Vannucci	CAMD, Department of Physics, Technical University of Denmark	Denmark
Lucas Cavalcante	Technical University of Denmark	Brazil
Mads-Peter Verner Christiansen	Aarhus University	Denmark
Malthe Bisbo	Aarhus University	Denmark
Marco Bragato	University of Basel	Switzerland
Mark Kamper Svendsen	DTU	Denmark
Mathias Dankl	EPFL	Switzerland
Megha Anand	Denmark Technical University	United States
Michael Statt	Stanford University	United States
Mihovil Bosnar	Ruđer Bošković Institute	Croatia
Mohammad Bahmani	Bremen Center for Computaional Materials Science	Germany
Morten Niklas Gjerding	DTU Physics	Denmark
Nan Zhang	Leibniz-Institut für Katalyse	Germany
Narges Atrak	University of Iceland	Iceland
Nathalie Vonrüti	University of Bern	Switzerland
Paavo Auvinen	University of Eastern Finland	Finland
Paulo André Gonçalves	Technical University of Denmark	Denmark
Peng Chen	Italian Institute of Technology	Italy
Pierre-Louis Lee	Scalian	France
Piotr de Silva	DTU Energy	Denmark
Raul Flores	Stanford University	United States
Rina Ibragimova	Aalto University	Finland
Robert Sandberg	Stanford University	United States
Rubén Soria Martínez	University of Strasbourg - CNRS	France
Rune Christensen	Technical University of Denmark	Denmark
Samantha Hood	Imperial College London	United Kingdom
Sanghoon Lee	Korea Atomic Energy Research Institute	South Korea
Sara Kelly	Stanford University	United States
Selwyn Hanselman	Leiden University	Netherlands
Shashi Bhusan Mishra	INDIAN INSTITUTE OF TECHNOLOGY MADRAS	India
Simone Manti	Technical University of Denmark	Denmark
Sindre Søpstad	University College of Southeast Norway	Norway
Spyridon Divanis	University of Copenhagen	Denmark
Steen Lysgaard	DTU Energy	Denmark
Stefan Heinen	Uni Basel	Switzerland
Sten Haastrup	CAMD, DTU	Denmark
Søren Ager Meldgaard	Aarhus University	Denmark
Teng Li	Leibniz-Institut für Katalyse	Germany
Thomas Bathelor	København Universitet	Denmark
Thomas Ludwig	Stanford University	United States
Thorbjørn Skovhus	Technical University of Denmark	Denmark
Thorsten Deilmann	CAMD, DTU	Denmark
Tim Würger	Helmholtz-Zentrum Geesthacht	Germany
Tugce Kutlusoy	Copenhagen University	Denmark
Uday Gajera	The Max-Planck-Institut für Eisenforschung GmbH	Germany
Unni Engedahl	Chalmers University of Technology	Sweden
Venkat Kapil	EPFL - IMX - COSMO	Switzerland
Venkata Surya Chaitanya Kolluru	University of Florida	United States
Vilhjálmur Ásgeirsson	University of Iceland	Iceland
Ville Korpelin	University of Jyväskylä	Finland
Vy Thi Hoang Nguyen	DTU Danchip	Denmark
Yanbing Zhu	Stanford	United States
Young-Kwang Jung	Yonsei University	South Korea
Yun Zhao	Leibniz-Institut für Katalyse e. V	Germany
Zeyuan Tang	Aarhus University, Department of Physics and Astronomy	Denmark
Zhihong Wei	Leibniz-Institut für Katalyse e. V.	Germany

Speakers:

Anatole von Lilienfeld	University of Basel	Switzerland

Name	Name of University/Institution/Company	Country
Aron Walsh	Imperial College London	United Kingdom
Bjørk Hammer	Aarhus University/Dept of Physics and Astronomy	Denmark
Christopher Wolverton	Northwestern University	United States
Claudia Draxl	HU Berlin	Germany
Eberhard Gross	MPI of Microstructure Physics	Germany
Georg Kresse	University of Vienna, Faculty of Physics	Austria
Hannes Jonsson	University of Iceland	Iceland
Jan Rossmeisl	KU	Denmark
Jens Kehlet Nørskov	DTU	Denmark
Kieron Burke	UC Irvine	United States
Nicola Marzari	EPFL	Switzerland
Stefano Curtarolo	Duke University	United States
Thomas Bligaard	SLAC	United States
Yan Sun	Max Planck Institute for Chemical Physics of Solids	Germany
Local seniors:		
Jakob Schiøtz	DTU Fysik	Denmark
Karsten W. Jacobsen	DTU	Denmark
Kristian Sommer Thygesen	DTU Physics	Denmark
Tejs Vegge	Technical University of Denmark	Denmark
Thomas Olsen	DTU	Denmark
Computing staff:		
Jens Jørgen Mortensen	DTU Physics	Denmark
Mikkel Strange	DTU Physics	Denmark
Administration:		
Marianne Ærsøe	DTU Physics	Denmark

The CAMD Summer School
Electronic Structure Theory and Materials Design 2018

Program:

Sunday, August 12:
11:30-13:15 Registration and lunch
13:15-13:30 Welcome
13:30-14:30 Fundamentals of DFT and TDDFT (Hardy Gross)
14:30-15:00 Coffee break and check-in
15:00-16:00 Electronic structure tools: ASE and GPAW (Jakob Schiøtz)
16:00-18:00 Computer exercises
19:00 Dinner

Monday, August 13:
07:00-09:30 Breakfast
09:30-10:30 Rate Theory (Hannes Jonsson)
10:30-11:00 Coffee break
11:00-12:00 Computational Design in Catalysis (Jens Nørskov)
12:00-13:30 Lunch
13:30-14:30 Structures and Reactions at Surfaces (Bjørk Hammer)
14:30-15:00 Coffee break
15:00-16:00 Electrochemistry (Jan Rossmeisl)
16:00-18:00 Computer exercises
18:00 Poster session with sandwiches

Tuesday, August 14:
07:00-09:30 Breakfast
09:30-10:30 Many-Body Perturbation Theory (Georg Kresse)
10:30-11:00 Coffee break
11:00-12:00 Theoretical Spectroscopy (Claudia Draxl)
12:00-13:30 Lunch
13:30-14:30 2D materials (Nicola Marzari)
14:30-15:00 Coffee break
15:00-16:00 Excitations in 2D materials (Kristian S. Thygesen)
16:00-18:00 Computer exercises
19:00 Dinner

Wednesday, August 15:
07:00-09:00 Breakfast
09:00-10:00 Machine Learning Basics (Karsten W. Jacobsen)
10:00-10:30 Coffee break
10:30-11:30 Machine Learning and Materials Science (Christopher Wolverton)
11:30-12:30 Lunch
12:30-13:30 Machine Learning and Chemistry (Anatole von Lilienfeld)
13:30-14:30 Machine Learning and Structural Search (Bjørk Hammer)
Rest of the day: Excursion and social dinner

Thursday, August 16:

07:00-09:30	Breakfast
09:30-10:30	Spin-orbit physics (Thomas Olsen)
10:30-11:00	Coffee break
11:00-12:00	Topological States of Matter (Yan Sun)
12:00-13:30	Lunch
13:30-14:30	Materials Informatics (Thomas Bligaard)
14:30-15:00	Coffee break
15:00-16:00	Discovery of Novel Electronic Materials (Stefano Curtarolo)
16:00-18:00	Computer exercises
19:00	Dinner

Friday, August 17:

07:00-09:30	Breakfast
09:30-10:30	Materials Modelling for Solar Cells: Perovskites and Beyond (Aron Walsh)
10:30-11:00	Coffee break
11:00-12:00	Batteries (Tejs Vegge)
12:00-13:30	Lunch
13:30-14:30	The Future of DFT (Kieron Burke)
14:30-15:00	Closing remarks and evaluation