Report

Hands-on Tutorial on *Ab Initio* Molecular Simulations: Toward a First-Principles Understanding of Materials Properties and Functions

Monday, June 22 - Wednesday, July 1, 2009, Harnack House, Berlin, Germany

Organizers: Volker Blum, Karsten Reuter, and Matthias Scheffler

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Density functional theory (DFT) today is a powerful framework for many aspects of electronic structure theory. A whole field, "computational materials science", is now concerned with the prediction of materials properties (molecules, liquids, solids, …) based on the principles of quantum mechanics alone. Developments "beyond" the realm of traditional DFT are rapid, including the ground state (new functionals, the RPA, inclusion of quantum chemical methods, quantum Monte Carlo), excited states (*GW*), or "multiscale" methods towards large length- and timescales.

This ten-day workshop taught in a tutorial manner the background and state-of-the-art of "DFT and beyond" in electronic structure theory. This included specifically the quality, power, and limits of present-day treatments of exchange and correlation. An additional focus addressed issues of multiscale modeling from first principles, which involves the linkage of DFT with thermodynamics, continuum descriptions, and statistical mechanics.

The tutorial was organized in a two-pronged format, enabling participants to gain an in-depth understanding of concepts and methods. Morning lectures, with keynotes by international leaders in the field and special-focus talks by local experts, were combined with practical computer exercises in the afternoons, led by local tutors. Here student teams tackled case studies representing real research tasks as well as – enthusiastically working in the lab often until late in the evenings – a collaborative, all-teams project (structural phases of transition metals). This format proved most effective in providing comprehensive training and intense scientific interaction. With nearly one hundred participants overall this workshop attests to the high demand for advanced training in the field. In fact, out of the many highly qualified applicants "only" the top ~70% could eventually be admitted as students to keep the workshop at a manageable size.

The program of the workshop is summarized below. Detailed information, including the lecture material, can be found on the tutorial's permanent website http://www.fhi-berlin.mpg.de/th/Meetings/DFT-workshop-Berlin2009/.

Berlin, September 2009

Volker Blum
Matthias Scheffler

Program

Keynote lectures are 50 minutes long plus ten minutes for discussion. The talks will take place in the Harnack House "Goethe-Saal". All practical sessions will be held in the lecture theater ("Hörsaal") of the nearby Fritz Haber Institute.

Poster Session – all participants are asked to present their research in the poster session (location: Harnack House "Wintergarten"). Poster boards are 1.15 m wide and 1.45 m high.

Monday, June 22	**Electronic structure theory**	
11:00		Registration
14:30 - 14:45		Welcome & Introductory Remarks
14:45 - 15:45	Matthias Scheffler, *Berlin* (Keynote 1)	Electronic structure theory & DFT: Status, achievements, challenges
15:45 - 16:45	E.K.U. Gross, *Berlin* (Keynote 2)	Electronic structure frontiers: Time dependence, excitations, electron-phonon coupling etc.
16:45 - 17:00	**Coffee break**	
17:00 - 19:00	Poster parade	(2 min./participant)
19:00 - 20:00	Break	
20:00	Barbecue	Harnack House

Tuesday, June 23	**Basics: Making DFT work**	
From 06:30 - 09:00	**Breakfast**	Harnack House
09:00 - 10:00	Kieron Burke, *Irvine* (Keynote 3)	Ground-state exchange and correlation
10:00 - 11:00	Volker Blum, *Berlin* (Keynote 4)	Practical electronic structure theory: Overview
11:00 - 11:30	**Coffee break**	
11:30 - 12:30	Ralf Gehrke, *Berlin* (Keynote 5)	Making electronic structure theory work: Self-consistency, total energy derivatives (forces), structure optimization
12:30 - 14:00	**Lunch**	FU Mensa
14:00 - 18:00	Practical session 1	Basics of electronic structure theory Team: Ralf Gehrke, Alexandre Tkatchenko
18:30 - 19:30	**Dinner**	FU Mensa
19:30	Participant poster session, Harnack House "Wintergarten"	

Wednesday, June 24	**Periodic systems**	
From 06:30 - 09:00	**Breakfast**	Harnack House
09:00 - 10:00	Peter Kratzer, *Duisburg* (Keynote 6)	Basics of DFT applications to solids and surfaces
10:00 - 11:00	Annabella Selloni, *Princeton* (Keynote 7)	Overview of plane wave methods
11:00 - 11:30	**Coffee break**	
11:30 - 12:30	Ricardo Gómez-Abal, *Berlin* (Keynote 8)	The all-electron "gold standard": Augmented plane wave methods
12:30 - 14:00	**Lunch**	FU Mensa
14:00 - 18:00	Practical session 2	Solids and surfaces Team: Paula Havu, Mina Yoon
18:30 - 19:30	**Dinner**	FU Mensa
20:00 - 22:00	Extra computer time with tutors on hand	

Thursday, June 25	**Exchange and correlation**	
From 06:30 – 09:00	**Breakfast**	Harnack House
09:00 - 10:00	Xinguo Ren, *Berlin* (Keynote 9)	Beyond LDA and GGA - Hartree-Fock, hybrid functionals, MP2, and RPA in FHI-aims: A numerical orbital practice
10:00 - 11:00	Alexandre Tkatchenko, *Berlin* (Keynote10)	Understanding van der Waals interactions – status and current solutions
11:00 - 11:30	**Coffee break**	
11:30 - 12:30	Dario Alfè, *London* (Keynote 11)	Quantum Monte Carlo
12:30 - 14:00	**Lunch**	FU Mensa
14:00 - 18:00	Practical session 3	"Participant research project" Team: Aloysius Soon, Matthias Scheffler The results will be presented in an evening talk on Tuesday by Matthias Scheffler
18:30 - 19:30	**Dinner**	FU Mensa
20:00 - 22:00	Extra computer time with tutors on hand	

Friday, June 26	**Structure and dynamics**	
From 06:30 – 09:00	**Breakfast**	Harnack House
09:00 - 10:00	Matt Probert, *York* (Keynote 12)	Structure prediction in materials science
10:00 - 11:00	Michele Parrinello, *Manno* (Keynote 13)	Molecular dynamics
11:00 - 11:30	**Coffee break**	
11:30 - 12:30	Gert von Helden, *Berlin* (Keynote 14)	Fingerprinting molecules: Vibrational Spectroscopy, Experiment and Theory
12:30 - 14:00	**Lunch**	FU Mensa
14:00 - 18:00	Practical session 4	Molecular dynamics Team: Mariana Rossi, Luca Ghiringhelli
18:30 - 19:30	**Dinner**	FU Mensa
20:00 - 22:00	Extra computer time with tutors on hand	
Saturday, June 27		
From 06:30 – 09:00	**Breakfast**	Harnack House
09:00 - 12:00	Time for participant research project	
14:00 - 20:00	Conference excursion (incl. dinner)	
Sunday, June 28		
From 07:00 – 10:00	**Breakfast**	Harnack House
All day	Time for participant research project	
Monday, June 29	**Spectroscopy**	
From 06:30 – 09:00	**Breakfast**	Harnack House
09:00 - 10:00	Martin Wolf, *Berlin* (Keynote 15)	Why excited states matter
10:00 - 11:00	Karsten Reuter, *Berlin* (Keynote 16)	Microscopy and spectroscopy: DFT-based analysis of surface science techniques
11:00 - 11:30	**Coffee break**	
11:30 -12:30	Patrick Rinke, *Santa Barbara* (Keynote 17)	GW-quasiparticle calculations
12:30 - 14:00	**Lunch**	FU Mensa
14:00 - 18:00	Practical session 5	Surfaces, core-level shifts, and STM images Team: Sergey Levchenko, Karsten Reuter
18:30 – 19:30	**Dinner**	FU Mensa
20:00 – 22:00	Extra computer time with tutors on hand	

Tuesday, June 30	**Frontiers I: The real electrons (exchange-correlation, transport, nano-electronics)**	
From 06:30 - 09:00	**Breakfast**	Harnack House
09:00 - 10:00	Ville Havu, *Helsinki* (Keynote 18)	Making electronic structure methods "scale": Large systems, (massively) parallel
10:00 - 11:00	Angel Rubio, *San Sebastian* (Keynote 19)	Response functions in low dimensional systems: from optics to transport
11:00 - 11:30	**Coffee break**	
11:30 - 12:30	Henning Riechert, *Berlin* (Keynote 20)	Impact of electronic structure theory in industry
12:30 - 14:00	**Lunch**	FU Mensa
14:00 - 18:00	Practical session 6	Solids: Phonons, Cv, thermal expansion Team: Felix Hanke, Martin Fuchs
18:30 - 19:30	**Dinner**	FU Mensa
20:00	Matthias Scheffler*, Berlin*	Evening talk at the Harnack House "Goethe-Saal"

Wednesday, July 1	**Frontiers II: Challenges for first-principles molecular simulations**	
From 06:30 – 09:00	**Breakfast**	Harnack House
09:00 - 10:00	Karsten Reuter, *Berlin* (Keynote 21)	*Ab initio* thermodynamics & Kinetic Monte Carlo
10:00 - 11:00	Horia Metiu, *Santa Barbara* (Keynote 22)	Problems in computational catalysis
11:00 - 11:30	**Coffee break**	
11:30 - 12:30	Roberto Car, *Princeton* (Keynote 23)	Challenges for first-principles molecular simulations
12:30	**Lunch** **& End of workshop**	FU Mensa