Research Networking Programmes

Science Meeting – Scientific Report

Scientific report (one single document in WORD or PDF file) should be submitted online within two months of the event. It should not exceed seven A4 pages.

Proposal Title: Hands-on workshop "Density-functional theory and beyond: Computational materials science for real materials"

Application Reference N°: 4605

1) Summary (up to one page)

From August 06 through 15, 2013, the Fritz Haber Institute (FHI) in Berlin and the International Centre for Theoretical Physics (ICTP) in Trieste organized a "Hands-On Workshop: Density Functional Theory and Beyond" in Trieste. The workshop convened a total of 107 participants from 20 countries, among them 35 lecturers and tutors as well as 72 student and postdoc participants, who had been selected from over 300 applicants. The workshop offered a broad introduction to computational materials science based on quantum-mechanical methods, ranging from the fundamentals (e.g., basic electronic structure theory, density functional theory, *ab initio* molecular dynamics) to advanced research topics at the forefront of the field. This material was presented in 24 keynote lectures (1 hour each) in morning sessions, as well as six all-afternoon tutorial sessions at the computer, and a weekend tutorial session. In addition, a poster session and poster parade allowed the participants to introduce themselves and their scientific interests to the other participants, speakers, and tutors. Overall, as organizers we were impressed by the motivated and focused group of participants that we were allowed to host during this event. The facilities at ICTP are a beautiful and extremely efficient setting for a hands-on computer workshop of this size, including its experienced staff, state-of-the-art technical capabilities for computer exercises and the ability to record all scientific events, which are now online at ICTP. We note that an article describing the workshop was also published online at
http://www.ictp.it/about-ictp/media-centre/news/2013/9/dft_workshop.aspx .

2) Description of the scientific content of and discussions at the event (up to four pages)

The workshop consisted of three broad parts: Basic concepts of electronic structure theory (August 6-8), advanced concepts including electronic structure, degrees of freedom or the nuclei, spectroscopy and multiscale models based on quantum-

mechanical input (August 9-14) and an "outlook day" featuring implications of the field in the "Materials Genome" context (US) and in industry.

Two overview lectures on the first day (Scheffler, Baroni) set the tone regarding electronic structure theory for ground-state and excited-state (spectroscopic) applications, followed by a poster parade with two-minute presentations each by the participants. On the second day, M. Casida presented an in-depth overview of electronic exchange-correlation treatments - the methodological centerpiece of the field - from a theoretical chemist's point of view. Lectures introducing the technical pieces that now form the standard foundation of the field in terms of powerful electronic structure code packages added to the introduction (Blum, Hofmann), and a first tutorial introduced these basic aspects - especially, the implications of different approximations to exchange and correlation - in terms of simple non-periodic molecules. As all other tutorials, this step was based on the FHI-aims code and supervised by approximately fifteen tutors and speakers from Berlin, all of whom were experienced in the handling of this code. The poster session brought together the entire conference on this evening, with posters remaining up for discussions (and being frequently used) during the entire remaining workshop period. August 8 was dedicated to periodic systems - the basic concepts (Bloch theorem, band structures and densities of state, etc.; Moll) as well as plane-wave based electronic structure approaches that are inherently periodic in nature (Gebauer, Draxl). The afternoon tutorial introduced periodic systems in practice, offering both basic exercises for participants not yet familiar with these concepts, as well as advanced steps (surface structure, magnetic systems) for participants with a prior background in these methods.

The second broad part of the workshop began on August 9 with in-depth lectures on electronic structure approaches beyond density functional theory (Levchenko and Neese), including an impressive sweep of quantum chemical approaches from the basics to linear-scaling coupled cluster theory (singles, doubles and perturbative triples, CCSD(T)) for very large systems by Neese. Another extremely active area is the application of DFT-based methods to the statistical mechanics and dynamics of the nuclei, with expert introductions to ab initio thermodynamic descriptions of solid materials (Neugebauer) as well as molecular dynamics (Rossi) and a tutorial on key basic aspects of molecular dynamics. The weekend featured hands-on sessions with tutors, during which participants chose their own small research projects, ranging from applications in their own fields to actual, hands-on programming experience for a scientific problem. The participants were, of course, not constrained to be present during these exercises, but an impressively large number did, making this a rewarding experience both for the participants and for the tutors.

Transport properties (Evers, Carbogno) and electronic excitations (Rinke, Appel) of molecules and solids formed the key areas covered on August 12, including a complete tutorial on Kubo-Greenwood based charge transport in solids from first principles (this is another "hot topic" with active development going on across the field). Statistical mechanics (Ghiringhelli) and the incorporation of nuclear motion beyond the classical approximation (Car) were key topics on August 13, together with an introduction to the extremely active topic of long-range dispersion interactions (Tkatchenko) and their proper incorporation into density functional theory. Electronic excitations as a tutorial topic picked up a theme from the previous day. Almost finally, an entire day was devoted to bringing quantum mechanical accuracy to larger scales, either directly (Haynes, linear scaling DFT) or by way of multiscale models (Behler, Kratzer). A tutorial on this topic was prepared by Gus Hart (BYU) in the afternoon of the same day, showing how a model Hamiltonian can be effectively and reliably set up based on quantum mechanical input.

The last day served as on outlook day, with a lecture on the Materials Genome (Hart), theory-led research at BASF (Rieger) and a culminating lecture on challenges addressed at BP (Ellen Williams, CSO, BP). This ended the workshop with a stimulating outlook for all participants. We note with some pride that the lecture room remained full up to the very end.

3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

We brought together an audience of bright and motivated young scientists from a global backdrop, both from developed countries and from (ICTP's core mission) the developing world. We are extremely fortunate to work in a field that offers ample perspectives for growth and unprecented scientific discoveries to its young scientists - both the ongoing growth of computational resources and the dedication of young scientists to push methods and algorithms further contribute to this growth. It is extremely pleasing to see that these basic insights are indeed being incorporated into in-house basic industrial science, as well as having already spawned some of the highest-cited papers in physics today.

It is the organizers' experience that many of the participants at our format of event (held since 1994 in a roughly biannual rhythm) are often scientists that stay in the field. Several of those that meet at such a focused school do form scientific bonds that may last for many years beyond. In fact, Blum (one of the organizers) participated in a much earlier event in Trieste, in 1999. Amazingly, his roommate at the time is now a Professor in Iran and an ICT fellow, who introduced his student to the 2013 workshop reported here.

It is of course hard to quantify the overall progress of the field in terms of its origin at workshops such as our own. Nonetheless, the opportunity to experience the vision of some of the leading experts of the field in a limited audience of focused, motivated (and, simply, friendly and welcoming) peers is a unique experience. Some of the material presented at the workshop was advanced enough to surprise even long-time experts in the field. At the same time, we believe that we have created a format that allowed every participant to learn starting from their own level, taking home valuable experiences (and research materials) to stimulate their work and ultimately propel forward the field itself.

4) Annexes 4a) and 4b): Programme of the meeting and full list of speakers and participants

Annex 4a: Programme of the meeting

Density functional theory and beyond: Computational materials science for real materials

Held at the Abdus Salam International Centre for Theoretical Physics (ICTP)
Trieste, Italy, August 06 - August 15, 2013

Workshop Program

This schedule is final, all lectures are for 50 min + 10 min discussion.

Poster dimensions: The poster board size is limited as 1.00 m (width) x 1.90 m (height). For example, A0 portrait format should work. We do not handle poster printing.

Program and Abstract Booklet: Program-and-Poster-Abstracts_HandsOnDFT2013.pdf

Tuesday, August 6: The Big Picture: Electronic Structure Theory		
9:00 - 11:30		Registration (outside Kastler lecture hall, Adriatico guest house) *Participants arriving later can still register in the Conference Secretariat's office at the Adriatico Guest House (Office No. 1, Lower Level 1) during the morning hours.*
14:30 - 14:45	Volker Blum, Ralph Gebauer	Introductory remarks
14:45 - 15:45	Matthias Scheffler	Electronic Structure Overview Lecture_1_Scheffler_HandsOnDFT2013.pdf
15:45 - 16:45	Stefano Baroni	Challenges Beyond Ground-State Electronic Structure Theory Lecture_2_Baroni_HandsOnDFT2013.pdf
16:45 - 17:15	*Coffee Break*	
17:15 - 19:00		Poster parade (2 min. talks by all participants)
19:00 - 22:00	*Welcome Reception*	
Wednesday, August 7: The Basics of DFT		
09:00 - 10:00	Mark Casida	Exchange and Correlation Lecture_3_Casida_HandsOnDFT2013.pdf
10:00 - 11:00	Volker Blum	Electronic Structure Theory in Practice I Lecture_4_Blum_HandsOnDFT2013.pdf
11:00 - 11:30	*Coffee Break*	

11:30 - 12:30	Oliver Hofmann	Electronic Structure Theory in Practice II Lecture_5_Hofmann_HandsOnDFT2013.pdf
12:30 - 14:00	*Lunch Break*	
14:00 - 18:00	Lydia Nemec, Oliver Hofmann	Practical Session 1: The basics of electronic structure theory Intro_Tutorial1_2013.pdf , Tutorial1_2013.pdf
18:00 - 19:00	*Break*	
19:00 - 22:00		Poster session for participants (posters will be up for the whole week)
Thursday, August 8: Periodic Systems: Basic Concepts for Solids and Surfaces		
09:00 - 10:00	Nikolaj Moll	Periodic Systems: Concepts Lecture_6_Moll_HandsOnDFT2013.pdf
10:00 - 11:00	Ralph Gebauer	The Plane-Wave Pseudopotential Method Lecture_7_Gebauer_HandsOnDFT2013.pdf
11:00 - 11:30	*Coffee Break*	
11:30 - 12:30	Claudia Draxl	The Augmented Plane Wave Method Lecture_8_Draxl_HandsOnDFT2013.pdf
12:30 - 14:00	*Lunch Break*	
14:00 - 18:00	Franz Knuth, Sergey Levchenko	Practical Session 2: Periodic Systems: Bulk Materials, Band Structures and Densities of States Intro_Tutorial2_2013.pdf , Tutorial2_2013.pdf
18:00 - 20:30	*Dinner Break*	
20:30 - 22:00		Extra computer time with tutors on hand
Friday, August 9: Beyond LDA and GGA: Correlation & Bringing Back the Nuclei (I)		
09:00 - 10:00	Sergey Levchenko	Beyond DFT for Extended Systems Lecture_9_Levchenko_HandsOnDFT2013.pdf
10:00 - 11:00	Frank Neese	Electron Correlation: State of the Art in Quantum Chemistry Lecture_10_Neese_HandsOnDFT2013.pdf
11:00 - 11:30	*Coffee Break*	
11:30 - 12:30	Jörg Neugebauer	"Real Materials": Ab Initio Thermodynamics
12:30 - 14:00	*Lunch Break*	
14:00 - 15:00	Mariana Rossi	Ab Initio Molecular Dynamics Lecture_12_Rossi_HandsOnDFT2013.pdf

15:00 - 18:00	Carsten Baldauf, Adriana Supady, Franziska Schubert, Mariana Rossi, Luca Ghiringhelli	Practical Session 3: *Ab initio* Molecular Dynamics Tutorial3_2013.pdf
18:00 - 20:30	*Dinner Break*	
20:30 - 22:00		Extra computer time with tutors on hand
Saturday, August 10		
09:00 - 12:30		Weekend research project with tutors on hand CS_Constrained-Relaxation.pdf CS_RPA-basis-sets.pdf CS_anharmonic-vibrations.pdf CS_embedding.pdf CS_harmonic-vibrations.pdf CS_minimum-energy-path.pdf , CS_minimum-energy-path.tgz CS_replica-exchange_MD.pdf , CS_replica-exchange_MD.tgz Microtutorial_PLUMED.pdf , Microtutorial_PLUMED.tgz Microtutorial_Surface-Phase-Diagram.pdf , Microtutorial_Surface-Phase-Diagram.tgz
14:00 -		Outing (with dinner)
Sunday, August 11		
all day		Weekend research project with tutors on hand
Monday, August 12: Spectroscopy and Transport		
09:00 - 10:00	Ferdinand Evers	Electronic Transport
10:00 - 11:00	Patrick Rinke	Many-Body and GW Lecture_14_Rinke_HandsOnDFT2013.pdf
11:00 - 11:30	*Coffee Break*	

11:30 - 12:30	Heiko Appel	TDDFT and Optical Properties Lecture_15_Appel_HandsOnDFT2013.pdf
12:30 - 14:00	*Lunch Break*	
14:00 - 15:00	Christian Carbogno	Charge and Heat Transport in Solids Lecture_16_Carbogno_HandsOnDFT2013.pdf
15:00 - 18:00	Karsten Rasim, Christian Carbogno	Practical Session 4: Charge Transport in Solids at Finite Temperatures Intro_Tutorial4_2013.pdf , Tutorial4_2013.pdf
18:00 - 20:30	*Dinner Break*	
20:30 - 21:00	N.N.	*Open Stage*: Summary of the weekend research project (Info-Lab)
21:00 - 22:00		Extra computer time with tutors on hand
Tuesday, August 13: Beyond LDA and GGA: Correlation & Bringing Back the Nuclei (II)		
09:00 - 10:00	Luca Ghiringhelli	From Ab Initio Molecular Dynamics to Statistical Mechanics Lecture_17_Ghiringhelli_HandsOnDFT2013.pdf
10:00 - 11:00	Alexandre Tkatchenko	Practical Approach to Dispersion Interactions Lecture_18_Tkatchenko_HandsOnDFT2013.pdf
11:00 - 11:30	*Coffee Break*	
11:30 - 12:30	Roberto Car	Quantum Nuclei Lecture_19_Car_HandsOnDFT2013.pdf
12:30 - 14:00	*Lunch Break*	
14:00 - 18:00	Fabio Caruso, Heiko Appel, Patrick Rinke	Practical Session 5: Excited State Formalisms Intro_Tutorial5_2013.pdf , Tutorial5_2013.pdf
18:00 - 20:30	*Dinner Break*	
20:30 - 22:00		Extra computer time with tutors on hand
Wednesday, August 14: Large Scale and Multiscale		
09:00 - 10:00	Peter Haynes	Linear Scaling DFT Lecture_20_Haynes_HandsOnDFT2013.pdf
10:00 - 11:00	Jörg Behler	Coarse-graining potential energy surfaces from ab initio data using artificial neural networks Lecture_21_Behler_HandsOnDFT2013.pdf
11:00 - 11:30	*Coffee Break*	

11:30 - 12:30	Peter Kratzer	Coarse-Graining Time and Space: Kinetic Monte Carlo Lecture_22_Kratzer_HandsOnDFT2013.pdf
12:30 - 14:00	*Lunch Break*	
14:00 - 18:00	Gus Hart, Conrad Rosenbrock, Björn Bieniek	Practical Session 6: Multiscale Intro_Tutorial6_2013.pdf , Tutorial6_2013.pdf
18:00 - 20:30	*Dinner Break*	
20:30 - 22:00		Extra computer time with tutors on hand
Thursday, August 15: Towards Real-World Applications		
09:00 - 10:00	Gus Hart	Deciphering the Materials Genome Lecture_23_Hart_HandsOnDFT2013.pdf
10:00 - 11:00	Michael Rieger	Computational Materials Science at BASF Lecture_24_Rieger_HandsOnDFT2013.pdf
11:00 - 11:30	*Coffee Break*	
11:30 - 12:30	Ellen D. Williams	Frontiers for Basic Science (and Modelling) in Industry
12:30 - 14:00	*Lunch Break and end of the workshop*	

For reference, the program and tutorials offered at past hands-on workshops can be found at the following links:

Hands-On workshop 2011 in Berlin

Hands-On workshop 2009 in Berlin

Annex 4b: Full list of speakers and participants

The Abdus Salam International Centre for Theoretical Physics

Activity SMR.2475

Density-Functional Theory and Beyond: Computational Materials Science for Real Materials

A Hands-on Workshop and Tutorial

6 - 15 August 2013
ICTP, Trieste, Italy

Organizers:

Carsten Baldauf, Volker Blum, Matthias Scheffler - **Fritz Haber Institute (FHI), Berlin, Germany**
Ralph Gebauer - **the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy**

Co-sponsors:

Workshop websites at ICTP and FHI:

http://agenda.ictp.it/smr.php?2475 and *http://th.fhi-berlin.mpg.de/sitesub/meetings/DFT-workshop-2013/*

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