Final report

Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals 2012

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1 Summary

From August 28-31, 2012, we convened a workshop on electronic structure theory based on localized orbital basis sets, specifically numeric atom-centered basis functions, in Berlin, Germany. In electronic structure theory, these methods enjoy great and increasing popularity in a wide range of frameworks today (to name but a few examples: The Siesta code, the DMol^3 code, the FPLO code, the Conquest code, the ONETEP code, the FHI-aims code, and many others, as well as the traditional Gaussian-type orbital codes of quantum chemistry). A core focus of our workshop were scientific developments centered around the Fritz Haber *ab initio* molecular simulations (FHI-aims) code that originated in Berlin a few years ago. The workshop thus doubled as the "FHI-aims Developers' and Users' Meeting" 2012. Similar to an earlier event in 2010, it was our express intent to include participants from a wider background and related projects, a goal that was reflected in the mix of accepted participants.

We were able to accommodate a maximum of sixty participants at our workshop. In fact, the demand was higher, but a limit was imposed by the computer facilities at our disposal. The core program consisted of eighteen invited lectures, a poster session with 22 contributions, and three so-called "Hands-On discussion" sessions held in the afternoons. Especially the Hands-On discussions are a signature feature of our workshop format. Instead of following a traditional talk/discussion format, these afternoon sessions brought participants together in small or large groups to discuss particular topics of interest, with computers on-site if needed. Some topics were suggested by the organizers, but a key goal was to let participants determine their own topics interests, including the possibility to cover entirely different (related) areas. Each afternoon also offered one specific topic that was formally prepared as a computer tutorial for interested participants. Our experiences with this discussion format are excellent: The participants stayed on topic in motivated discussion groups throughout the conference site. We were fortunate to have the logistical support of the CECAM "SCM" node in Berlin, which helped us with a computer room, a seminar room, a comfortable coffee and posters session space with tables and an outside patio, giving us enough room to form individual discussion sessions in close proximity to one another. In addition, a large lecture theatre nearby provided the setting for the formal invited talks.

Overall, we encountered a lively group of participants that embraced the discussion and talk opportunities throughout the meeting with even more enthusiasm than the organizers could have hoped for. Details are given in the following sections.

2 Description of the scientific content of and discussion at the event

The program was split into four morning sessions with invited talks, one evening poster session, and three afternoon "Hands-On Discussion" sessions with computers on site, including three separate tutorial topics that had been prepared with considerable effort by external speakers.

In order to allow the participants to arrive on the day of the event, the first-day program consisted of two talks: First, a welcome and overview of recent electronic structure developments realized in the FHI-aims code ("State of FHI-aims"; Volker Blum, Berlin), and second, a presentation on arguably one of the most-wanted features in current electronic structure theory: Hartree-Fock and screened Hartree-Fock like exchange for hybrid functionals in Bloch-periodic systems (solids, surfaces, nanowires etc.; Sergey Levchenko, Berlin). The afternoon program featured a presentation on the computation of phonons in solids (Jörg Meyer, Munich), followed by the afternoon Hands-On Session and evening poster session (see below).

Over the following days, the program covered a broad range of current topics in electronic structure theory:

- Scalable linear algebra (Bruno Lang, Wuppertal)
- Molecular transport (Paula Havu, Espoo; Alexej Bagrets, Karlsruhe)
- Excited-state formalisms beyond traditional G_0W_0 approaches (Xinguo Ren, Fabio Caruso, Berlin)
- Molecular dynamics based statistical mechanics from first principles (Christian Carbogno, Santa Barbara; Mariana Rossi, Berlin; Davide Branduardi, Frankfurt; Karsten Reuter, Munich)
- Structure prediction (Scott Woodley, London)
- New functionals for more accurate first-principles descriptions of molecules and materials (Noa Marom, Austin; Igor Ying Zhang, Berlin; Eduardo Fabiano, Lecce; Ken Jordan, Pittsburgh; Alexandre Tkatchenko, Berlin)

Thus, a significant set of the current developments in electronic structure theory was addressed, in parts based on the FHI-aims frameworks, but also by participants with a significant background in other localized basis set methods (Bagrets, Ying Zhang, Fabiano, Jordan). The set of scientific topics included the specific area of expertise for each participant, but was broad enough to ensure that no one was an "expert for everything". The underlying common bracket, localized basis sets as the method, ensured a common language. We also benefitted significantly from the mix of some senior researchers in the field and many Ph.D. students and postdoctoral researcher with a direct, active interest in the topics.

The afternoon "Hands-On Discussions" each offered either a prepared tutorial on a specific topic with computers, or the participation in one of several on-site scientific discussion groups with a common interest. The tutorials were prepared by invited experts on three different topics: Phonon calculations in the "phonopy" framework and heat transport in solids (Jörg Meyer, Munich; Christian Carbogno, Santa Barbara); molecular transport calculations in the "aitranss" framework developed in Karlsruhe (Alexej Bagrets, Karlsruhe); and free energy calculations in the "plumed" framework (Davide Branduardi, Frankfurt; Luca Ghiringhelli, Berlin). In addition, the afternoon discussion topics ranged from simple technical topics to basic frontiers of our field: "New to FHI-aims", scalability with system size and computational hardware, frameworks for embedding of quantum-mechanically treated regions into external environments, pseudoization methods, molecular transport, molecular vibrations, technical aspects of phonon calculations, van der Waals interactions, "DFT beyond LDA and GGA", molecular dynamics, and strategies to achieve faster self-consistency. From the vantage point of the organizers, these discussions displayed a remarkable degree of self-organization, self-motivation and scientific quality on the part of the participants. What helped greatly was the mix of experts present on each topic (some acting as informal discussion leaders) and participants with an active need. If there is one regret of the organizers, it is not having been able to attend each of the parallel discussion sessions simultaneously.

The same spirit of active participation and discussion was displayed at the formal poster session, with

22 presented abstracts by participants, covering molecular science, problems in solid state physics, algorithmic problems and technical implementations alike. The posters remained on display for the entire duration of the workshop.

3 Assessment of the results and impact of the event on the future direction of the field

In summary, we are excited to have received perhaps the best reward that the organizers of a conference could wish for: A field of motivated participants that enthusiastically embraced all aspects of the program, with significant contributions from each one. Since the meeting was partially centered around the electronic structure framework FHI-aims, an immediate impact is the connection between scientists and developers from different locations and the resulting activity in the code itself. This, over time, will lead to numerous scientific opportunities in electronic structure applications, covering all the aspects mentioned above: High-level approaches, molecular dynamics, transport, statistical mechanics from first principles, and much more. Time will tell which and how many of the numerous threads begun at the meeting will mature: More robust frameworks for “external embedding” of quantum mechanical regions into surrounding fields, more accurate high-level electronic structure methods that are affordable for real (large) materials and molecular simulations, path integral formalisms to incorporate nuclear quantum effects into spectroscopy of hydrogen bonded systems, new approaches to van der Waals interactions, and many more.

4 Final program and list of participants

The final program and list of participants are attached on the following pages.

Program

Tuesday, August 28, 2012		
10:00 – 11:00	Registration	
11:00 – 11:15	Introductory Remarks	
11:15 – 11:50	Volker Blum	*State of FHI-aims*
11:50 – 12:25	Sergey Levchenko	*Hartree-Fock and hybrid functionals, periodic: Implementation and application to defects in doped MgO*
12:30 – 14:00	Lunch	
14:00 – 14:35	Jörg Meyer	*Phonons, FHI-aims, and the phonopy framework*
14:35 – 18:00	Jörg Meyer	*Tutorial: FHI-aims, phonopy, and heat transport*
	Christian Carbogno	and (in parallel)
	Participants	*Hands-On Discussion*
18:30 – 20:00	Dinner	
20:00 – 22:00	Poster Session	
Wednesday, August 29, 2012		
09:00 – 09:35	Bruno Lang	*Eigenvalue solvers – The ELPA Project and Beyond*
09:35 – 10:10	Paula Havu	*Graphane on SiO_2, transport in FHI-aims*
10:10 – 10:45	Alexej Bagrets	*Electron transport through molecular junctions and FHI-aims*
10:45 – 11:15	Coffee Break	
11:15 – 11:50	Xinguo Ren	*Beyond RPA and GW: renormalizated second-order perturbation theory for ground-state and excited-state calculations*
11:50 – 12:25	Fabio Caruso	*Self-consistent GW in FHI-aims*
12:30 – 14:00	Lunch	
14:00 – 16:00	Alexej Bagrets	*Tutorial: The aitranss transport framework*
		and (in parallel)
	Participants	*Hands-On Discussion*
16:00 – open end	Conference Outing and Dinner	
Thursday, August 30, 2012		
09:00 – 09:35	Christian Carbogno	*Heat transport from first principles in FHI-aims*
09:35 – 10:10	Mariana Rossi	*Ab initio molecular dynamics for biomolecular spectroscopy*
10:10 – 10:45	Davide Branduardi	*The PLUMED plug-in and free energy methods in electronic-structure-based molecular dynamics*
10:45 – 11:15	Coffee Break	
11:15 – 11:50	Karsten Reuter	*FHI-aims becomes embedded: QM/Me and water splitting*
11:50 – 12:25	Scott Woodley	*Structure prediction and solid solutions with evolutionary algorithms*
12:30 – 14:00	Lunch	
14:00 – 18:00	Davide Branduardi	*Tutorial: PLUMED and FHI-aims*
	Luca Ghiringhelli	and (in parallel)
	Participants	*Hands-On Discussion*
18:30 – 20:00	Dinner	

Friday, August 31, 2012		
09:00 – 09:35	Noa Marom	*Keeping Supercomputers Busy – Configuration Space Exploration and GW Calculations*
09:35 – 10:10	Igor Ying Zhang	*Development of the XYG3-type doubly-hybrid functionals*
10:10 – 10:45	Eduardo Fabiano	*Non-empirical semilocal functionals for improved performance in quantum chemistry and materials science*
10:45 – 11:15	Coffee Break	
11:15 – 11:50	Kenneth Jordan	*Exploring Intermolecular Correlation with SAPT, vdW-Corrected DFT, and Diffusion Monte Carlo Methods*
11:50 – 12:25	Alexandre Tkatchenko	*Van der Waals Interactions in Molecules, Solids, and Interfaces*
12:25 – 12:30	Closing remarks	
12:30	Lunch and end of workshop	

Participants

	Name	Institution	Participant type
1	Sadiq Abdul	Kaduna State University	Participant
2	Alberto Ambrosetti	Fritz Haber Institute	Participant
3	Balint Aradi	University of Bremen	Participant
4	Ido Azuri	Weizmann Institute of Science	Participant
5	Kurt Baarman	Aalto University School of Science	Participant
6	Alexej Bagrets	Karlsruher Institut für Technologie (KIT)	Speaker
7	Carsten Baldauf	Fritz Haber Institute	Participant
8	David Bende	MPI Chemische Physik fester Stoffe	Participant
9	Daniel Berger	TU München	Participant
10	Saswata Bhattacharya	Fritz Haber Institute	Participant
11	Robert Biele	European Theoretical Spectroscopy Facility (ETSF)	Participant
12	Björn Bieniek	Fritz Haber Institute	Participant
13	Volker Blum	Fritz Haber Institute	Speaker
14	Davide Branduardi	Max Planck Institute for Biophysics	Speaker
15	Christian Carbogno	University of California at Santa Barbara	Speaker
16	Fabio Caruso	Fritz Haber Institute	Speaker
17	Wael Chibani	Fritz Haber Institute	Participant
18	Jun-Hyung Cho	Hanyang University	Participant
19	Eduardo Fabiano	Nanoscience Institute of CNR	Speaker
20	Matthew Farrow	University College London	Participant
21	Luca Ghiringhelli	Fritz Haber Institute	Speaker
22	Hamidreza Hajiyani	ICAMS	Participant
23	Christopher Handley	Ruhr Universitat Bochum	Participant
24	Paula Havu	Research Associate at the Aalto University School of Science	Speaker
25	Ville Havu	Aalto University	Participant
26	Abdesalem Houari	University of Bejaia	Participant
27	Kenneth Jordan	University of Pittsburgh	Speaker
28	Yong-Hyun Kim	KAIST	Participant
29	Franz Knuth	Fritz Haber Institute	Participant
30	Peter Kratzer	University Duisburg-Essen	Participant
31	Bruno Lang	University of Wuppertal	Speaker
33	Florian Lazarevic	Fritz Haber Institute	Participant
33	Sergey Levchenko	Fritz Haber Institute	Speaker
34	Wenjin Li	CAS-MPG Partner Institute for Computational Biology	Participant
35	Xinzheng Li	Peking University	Participant
36	Andrew Logsdail	University College London	Participant
37	Luis Mancera	Universität Ulm	Participant
38	Noa Marom	The University of Texas at Austin	Speaker
39	Jörg Meyer	TU München	Speaker
40	Lydia Nemec	Fritz Haber Institute	Participant
41	Alim Ormeci	Max Planck Institute for Chem. Phys. of Solids	Participant
42	Diana Otalvaro	University of Twente	Participant
43	Zachary Pozun	University of Pittsburgh	Participant
44	Anthony Reilly	Fritz Haber Institute	Participant
45	Xinguo Ren	Fritz Haber Institute	Speaker
46	Karsten Reuter	TU München	Speaker
47	Patrick Rinke	Fritz Haber Institute	Participant
48	Mariana Rossi	Fritz Haber Institute	Speaker
49	Matthias Scheffler	Fritz Haber Institute	Participant

50	Franziska Schubert	Fritz Haber Institute	Participant
51	Jungho Shin	Korea Institute of Science and Technology	Participant
52	Alexey Sokol	University College London	Participant
53	Christian Spickermann	Atotech Deutschland GmbH	Participant
54	Alexandre Tkatchenko	Fritz Haber Institute	Speaker
55	Frank von Horsten	Atotech Deutschland GmbH	Participant
56	Vamsee Voora	University of Pittsburgh	Participant
57	Michael Walz	Karlsruher Institut für Technologie (KIT)	Participant
58	Chenchen Wang	University of Connecticut	Participant
59	Scott Woodley	University College London	Speaker
60	Jae Won Yang	Pohang University of Science and Technology	Participant
61	Ted Yu	University of California, Los Angeles	Participant
62	Igor Ying Zhang	Fritz Haber Institute	Speaker