Final report

Hands-On Tutorial: Density Functional Theory and Beyond, Concepts and Applications

1 Summary

We have organized and implemented a successful ten-day workshop on the concepts and applications behind modern electronic structure theory ("density functional theory and beyond") for computational materials science, held from July 12-21, 2011 at the Harnackhaus conference center and Fritz Haber Institute in Berlin, Germany. The workshop brought together an audience of more than 80 students and post-docs (108 including tutors from the Fritz Haber Institute) for 23 keynote lectures on the basics and selected advanced topics from the field, as well as six afternoon "hands-on" tutorials with computers and one weekend "hands-on" tutorial and research project. In addition, a "poster parade" on the first day and poster session on the second day provided each participant with an opportunity to introduce themselves and their work to the entire group, a key step to foster communication, information exchange, and ultimately, trust between the initially unconnected set of participants. Computer-based electronic structure theory from quantum-mechanical first principles is a rapidly growing field with a multitude of practical applications in condensed matter physics, materials science, nanoscience, (bio)molecular science, pharmacology, and other disciplines. The versatility of the field can also create a significant entry barrier especially for newly incoming researchers. The goal of the work was to provide such an entry into the field (by the more basic keynote lectures) and widening of scope (by the more advanced keynote lectures) for its entire audience.

Out of the more than 160 applicants, we were able to accommodate 80 external participants who formed a highly motivated, active audience not only in the tutorials, but also during the entire set of keynote lectures offered at the workshop. As in a previous event, we found the Harnackhaus conference center an excellent venue for the event, allowing to use the infrastructure of the nearby (50 metres) Fritz Haber Institute for the computational exercises rather efficiently. Aside from the actively tutored sessions, the computer facilities were available to all participants throughout the workshop, both for additional late-evening sessions with tutors on hand and for independent work. The showing even outside the regular afternoon and evening sessions amounted to a significant fraction of the participants—for example, we estimate that more than 50 % of the participants made regular use of the additional evening sessions. We also note that the workshop could not have been successful without the large efforts of the tutors at the Fritz Haber Institute (and, in two cases, externally at Brigham Young University in Provo, Utah) to create and perfect the specific, guided tutorials at the workshop.

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

Topically, the workshop was (roughly) split into three parts: a set of broader topics covering the scientific basics of the field (July 12-15), a weekend tutorial and research project (July 16 and 17), and a set of focused, advanced topics towards the frontiers of the field (July 18-21). Two overview lectures on July 12 covered the broader topics of electronic structure theory (Scheffler) and quantum chemistry (Sauer), followed by a "poster parade" that allowed each participant to introduce themselves and their research interest. The practical basics of density functional theory occupied the two first full days (July 13/14; Della Sala, Blum, Wieferink, Levchenko, Ambrosch-Draxl, Marsman), covering practical exchange-correlation approximations, and implementation aspects across three major code frameworks, including details of periodic systems, and capped by two introductory tutorials on these topics. July 15 covered some more advanced methodological foundations (time-dependent density functional theory, van der Waals interac-

tions, and many-body perturbation approaches; Gross, Tkatchenko, Ren), flanked by a tutorial introducing the “weekend research project” (July 16/17): Structure prediction of biologically relevant molecules (two amino-acid peptides) and the role of different exchange-correlation aspects in these systems. The second week was split as follows: Ground state and multiscale-type approaches (Ghiringhelli, Hart, Walsh; July 18), *ab initio* molecular dynamics and time-dependent phenomena (Car, Carbogno, Appel; July 19), electronic phenomena beyond ground-state approaches (Rinke, Biermann, Guo; July 20), and finally, some of the methodological frontiers of the field in real-world modelling settings (Reuter, Lampenscherf, Schulthess; July 21). July 18-20 saw corresponding tutorials that were directly integrated with the morning sessions and co-prepared by some of the speakers.

Based on the response of the participants, both to the actual keynote lectures (questions and discussions) and during the tutorials, we feel that we were able to maintain a high level of impact throughout the workshop. We believe that this success was helped by the mix of keynote speakers present, both local experts from FHI and high-profile, leading experts in the field (Sauer, Della Sala, Ambrosch-Draxl, Marsman, Gross, Hart, Walsh, Car, Biermann, Guo, Reuter, Schulthess). Likewise, the enormous efforts of the local tutorial organizers and tutors were essential to the success of the event. Without these elaborate preparations and active support by a large group of individuals (approx. 25) at FHI and elsewhere, the event could not have been successful.

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

The field of electronic structure theory is rather large today. Yet, aside from a small set of common basics, much of the field is not part of university curricula even at the graduate level in our experience. Based on the response from the participants, we believe that our attempt to link an in-depth introduction to the methodological basics with an ambitious range of advanced topics at the forefront of the field was a success. The impact of this event can perhaps be gauged in relation to past events — the workshop format in question happens since 1994 in intervals of roughly every two years, at FHI. The fact that 160 participants applied despite strong competition from parallel, unrelated workshops at a European scale within the same time frame shows, in our opinion, the need for comprehensive events such as ours more than anything else.

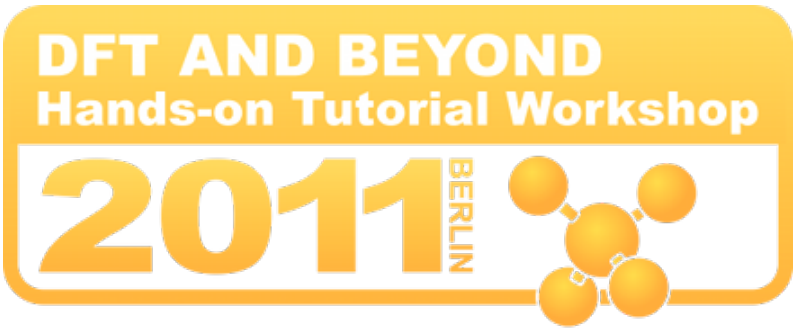
Apart from the discussions and tutorials held at the workshop, the results are available permanently on the world-wide web at:

`http://www.fhi-berlin.mpg.de/th/Meetings/DFT-workshop-Berlin2011/`

including links to all presentation slides and tutorial materials used at the workshop. We hope to have brought together, through our workshop, a diverse group of motivated researchers that are now coming into the field. In our experience, some of the ties formed at such events can last across significant parts of scientific careers, and instill long-term ideas in minds that are still fresh and unbiased enough to see them through. The goal of this workshop was to provide support to future researchers willing to make an impact in the field, and we hope that this first step was a success.

4 Final program and list of participants

The final conference program and list of participants are attached to this report on the following pages.



Hands-on Tutorial Workshop 2011 on Ab Initio Molecular Simulations: Toward a First-Principles Understanding of Materials Properties and Functions

Berlin, July 12 - 21, 2011

Workshop programme

Keynote lectures: 50 minutes long, leaving 10 minutes for discussions.
Poster size: width = 1.15 m, height = 1.45 m

Tuesday, July 12: The Big Picture: Electronic Structure Theory		
11:30-14:30	Harnackhaus (Lobby)	Registration
14:30-14:45	Harnackhaus (Goethesaal)	Introductory remarks
14:45-15:45	Harnackhaus (Goethesaal)	Matthias Scheffler (FHI Berlin) - Computational materials sciences from first principles: Status, achievements, challenges
15:45-16:45	Harnackhaus (Goethesaal)	Joachim Sauer (HU Berlin) - Quantum Chemistry and wave function based methods
16:45-17:15	Harnackhaus	Break
17:15-20:00	Harnackhaus (Goethesaal)	Poster parade (2 min. talks by all participants)
20:00-22:00	Richard-Willstätter-Haus (FHI)	Welcome Dinner
Wednesday, July 13: The Basics of Density Functional Theory		
6:30-9:00	Harnackhaus	Breakfast
9:00-10:00	Harnackhaus (Goethesaal)	Fabio Della Sala (NNL, Lecce) - XC functionals for the ground state
10:00-11:00	Harnackhaus (Goethesaal)	Volker Blum (FHI Berlin) - The nuts and bolts of electronic structure theory: basis sets, grids, relativity etc.
11:00-11:30	Harnackhaus	Break
11:30-12:30	Harnackhaus (Goethesaal)	Jürgen Wieferink (FHI Berlin) - The nuts and bolts of electronic structure theory (II): Self-consistency, gradients, relaxation and vibrations
12:30-14:00	Mensa (Freie Universität)	Lunch
14:00-18:00	FHI (Lecture Hall)	Practical session 1 - The basics of electronic structure theory (V. Atalla, O. Hofmann, S. Levchenko), presentation, instructions

18:30-20:00	Mensa (Freie Universität)	Dinner
20:00-22:00	Harnackhaus (Wintergarten)	Poster session for participants (posters will be up for the whole week)
Thursday, July 14: Periodic Systems		
6:30-9:00	Harnackhaus	Breakfast
9:00-10:00	Harnackhaus (Goethesaal)	Sergey Levchenko (FHI Berlin) - Basics for periodic systems
10:00-11:00	Harnackhaus (Goethesaal)	Claudia Ambrosch-Draxl (Uni Leoben) - LAPW and related methods: the example of the Exciting code
11:00-11:30	Harnackhaus	Break
11:30-12:30	Harnackhaus (Goethesaal)	Martijn Marsman (Uni Wien) - Plane wave methods, pseudopotentials, and PAW: the example of the VASP code
12:30-14:00	Mensa (Freie Universität)	Lunch
14:00-18:00	FHI (Lecture Hall)	Practical session 2 - Periodic systems: Solids, surfaces, band structure and reconstruction (J. Wieferink, L. Nemec), presentation, instructions
18:30-20:00	Mensa (Freie Universität)	Dinner
20:00-22:00	FHI (Lecture Hall)	Extra computer time with tutors on hand
Friday, July 15: Beyond LDA/GGA		
6:30-9:00	Harnackhaus	Breakfast
9:00-10:00	Harnackhaus (Goethesaal)	Hardy Gross (MPI Halle) - XC beyond static DFT
10:00-11:00	Harnackhaus (Goethesaal)	Alexandre Tkatchenko (FHI Berlin) - Approaches to van der Waals
11:00-11:30	Harnackhaus	Break
11:30-12:30	Harnackhaus (Goethesaal)	Xinguo Ren (FHI Berlin) - Beyond LDA and GGA in practice
12:30-14:00	Mensa (Freie Universität)	Lunch
14:00-18:00	FHI (Lecture Hall)	Practical session 3 - Weekend research project (beginning): Conformational space and energetics of (bio)molecules: Physical concepts and performance of DFT-based and correlated methods (A. Tkatchenko, C. Baldauf, M. Ropo), presentation, instructions
18:30-20:00	Mensa (Freie Universität)	Dinner
20:00-22:00	FHI (Lecture Hall)	Extra computer time with tutors on hand
Saturday, July 16		
6:30-9:30	Harnackhaus	Breakfast
9:00-13:00	FHI (Lecture Hall)	Weekend research project with tutors on hand
14:00-	Berlin	Excursion (open end, see separate schedule)
Sunday, July 17		
7:00-10:00	Harnackhaus	Breakfast
all day	FHI (Lecture Hall)	Weekend research project with tutors on hand (incl. light "working lunch" at the lecture hall)
18:30-20:00	Harnackhaus	"Working Dinner"

Monday, July 18: Ab initio Thermodynamics		
6:30-9:00	Harnackhaus	Breakfast
9:00-10:00	Harnackhaus (Goethesaal)	Elizabeth C. Beret / Luca Ghiringhelli (FHI Berlin) - Ab initio atomistic thermodynamics
10:00-11:00	Harnackhaus (Goethesaal)	Gus Hart (Brigham Young University) - Cluster expansion and multiscale modelling
11:00-11:30	Harnackhaus	Break
11:30-12:30	Harnackhaus (Goethesaal)	Aron Walsh (UCL London) - Modelling materials and processes for solar cells
12:30-14:00	Mensa (Freie Universität)	Lunch
14:00-18:00	FHI (Lecture Hall)	Practical session 4 - Multiscale modeling of configurational energetics (G. Hart, V. Blum, N. Richter), presentation, instructions
18:30-20:00	Mensa (Freie Universität)	Dinner
20:00-20:30	FHI (Lecture Hall)	Matthias Scheffler (FHI) - One hundred years of science in Dahlem: History of the FHI and of the MPG
20:30-22:00	FHI (Lecture Hall)	Extra computer time with tutors on hand
Tuesday, July 19: Molecular Dynamics and Time-Dependent DFT		
9:00-10:00	Harnackhaus (Goethesaal)	Roberto Car (Princeton) - Ab initio molecular dynamics: from the basics up to quantum effects
10:00-11:00	Harnackhaus (Goethesaal)	Christian Carbogno (FHI Berlin and UC Santa Barbara) - Thermostats and thermal transport in solids
11:00-11:30	Harnackhaus	Break
11:30-12:30	Harnackhaus (Goethesaal)	Heiko Appel (FHI Berlin) - Introduction to real-space, linear-response, and time-dependent methods: the example of the Octopus code
12:30-14:00	Mensa (Freie Universität)	Lunch
14:00-18:00	FHI (Lecture Hall)	Practical session 5 - Phonons, molecular dynamics and free energies for solids (C. Carbogno, L. Ghiringhelli, M. Rossi), presentation part 1, presentation part 2, instructions
18:30-20:00	Mensa (Freie Universität)	Dinner
20:00-22:00	FHI (Lecture Hall)	Extra computer time with tutors on hand
Wednesday, July 20: Spectroscopy and Transport		
6:30-9:00	Harnackhaus	Breakfast
9:00-10:00	Harnackhaus (Goethesaal)	Patrick Rinke (FHI Berlin) - Excited states and GW/BSE
10:00-11:00	Harnackhaus (Goethesaal)	Silke Biermann (Ecole Polytechnique, Palaiseau) - Strong correlation - what is it, and how to tackle it (DMFT)
11:00-11:30	Harnackhaus	Break
11:30-12:30	Harnackhaus (Goethesaal)	Hong Guo (McGill University) - Basics of electronic transport
12:30-14:00	Mensa (Freie Universität)	Lunch
14:00-18:00	FHI (Lecture Hall)	Practical session 6 - Computational spectroscopy (H. Appel, P. Rinke, F. Caruso), presentation, instructions
18:30-20:00	Mensa (Freie Universität)	Dinner

20:00-22:00	FHI (Lecture Hall)	Extra computer time with tutors on hand
Thursday, July 21: Electronic Structure Frontiers		
6:30-9:00	Harnackhaus	Breakfast
09:00-10:00	Harnackhaus (Goethesaal)	Karsten Reuter (TU München) - Towards first-principles chemical engineering
10:00-11:00	Harnackhaus (Goethesaal)	Stefan Lampenscherf (Siemens AG, Corporate Technology) - Electronic structure theory in industry
11:00-11:30	Harnackhaus	Break
11:30-12:30	Harnackhaus (Goethesaal)	Thomas Schulthess (ETH Zürich) - Electronic structure theory at the petascale and beyond
12:30-14:00	Mensa (Freie Universität)	Lunch and End of Workshop

Density Functional Theory and Beyond 2011 - Participant List

	Name	Institution	Participant type
1	Abdul, Sadiq	Kaduna State University, Nigeria	Student
2	Ambrosch-Draxl, Claudia	University of Leoben, Austria	Speaker
3	Ambrosetti, Alberto	Padova University, Italy	Postdoc
4	Appel, Heiko	Fritz Haber Institute, Berlin, Germany	Organizer
5	Bakulin, Alexander	Tomsk State University, Russia	Student
6	Baldauf, Carsten	Fritz Haber Institute, Berlin, Germany	Postdoc / Tutor
7	Baumgärtel, Michael	German Research School for Simulation Sciences, Jülich	Student
8	Berger, Daniel	Technical University of Munich, Germany	Student
9	Bernal Villamil, Ivan	Instituto de Ciencia de Materiales (CSIC), Madrid, Spain	Student
10	Bienek, Björn	Fritz Haber Institute, Berlin, Germany	Student / Tutor
11	Biermann, Silke	Ecole Polytechnique Palaiseau, France	Speaker
12	Biller, Ariel	Weizmann Institute of Science, Rehovot, Israel	Student
13	Birenbaum, Yael	Trinity College, Dublin, Ireland	Student
14	Blum, Volker	Fritz Haber Institute, Berlin, Germany	Organizer
15	Brandimarte Mendonca, Pedro	University of Sao Paulo, Brazil	Student
16	Camarillo Cisneros, Javier	Centro de Investigacion en Materiales Avanzados, Chihuahua, Mexico	Student
17	Car, Roberto	Princeton University, USA	Speaker
18	Carbogno, Christian	University of California, Santa Barbara, USA	Speaker
19	Caruso, Fabio	Fritz Haber Institute, Berlin, Germany	Student / Tutor
20	Casadei, Marco	Fritz Haber Institute, Berlin, Germany	Student / Tutor
21	Chen, Yue	Chinese Academy of Sciences, Shenyang	Postdoc
22	Cheng, Jun	Cambridge University, England	Postdoc
23	Chibani, Wael	Fritz Haber Institute, Berlin, Germany	Student / Tutor
24	Chutia, Sucismita	Fritz Haber Institute, Berlin, Germany	Postdoc / Tutor
25	da Silva, Estelina	University of Coimbra, Portugal	Student
26	Daon, Shauli	Weizmann Institute of Science, Rehovot, Israel	Student
27	Dasari, Prasad	MPI f. Solid State Research, Stuttgart, Germany	Postdoc
28	Della Sala, Fabio	Universita del Salento, Lecce, Italy	Speaker
29	Dey, Gangotri	Tyndall National Institute, Ireland	Student
30	Dolui, Kapildeb	Trinity College, Dublin, Ireland	Postdoc
31	Dostert, Catherine	Heinrich Heine University, Düsseldorf, Germany	Student
32	Dymkowski, Krzysztof	Trinity College, Dublin, Ireland	Student
33	Erikat, Ihsan	Jerash University, Jordan	Postdoc
34	Ferri, Nicola	Fritz Haber Institute, Berlin, Germany	Student
35	Fidder, Hendrik	Max Born Institute, Berlin, Germany	Postdoc
36	Filimonov, Sergey	Tomsk State University, Russia	Postdoc
37	Gallet, Gregoire	EPFL, Lausanne, Switzerland	Student
38	Gallino, Federico	Universitá degli Studi Milano-Bicocca, Italy	Student
39	Ghiringhelli, Luca	Fritz Haber Institute, Berlin, Germany	Speaker
40	Go, Anna	University of Bialystok, Poland	Postdoc
41	Gobre, Vivekanand	Fritz Haber Institute, Berlin, Germany	Student / Tutor
42	Golesorkhtabar, Rostam	University of Leoben, Austria	Student
43	Graziano, Gabriella	University College London, England	Student
44	Gross, Eberhard	MPI for Microstructure Physics, Halle, Germany	Speaker
45	Gruber, Mathis	Fritz Haber Institute, Berlin, Germany	Student
46	Güller, Francisco	Comisión Nacional de Energía Atómica, Bariloche, Argentina	Student
47	Gunst, Tue	Technical University of Denmark, Copenhagen	Student
48	Guo, Chungsheng	Fritz Haber Institute, Berlin, Germany	Postdoc / Tutor

49	Guo, Hong	McGill University, Montreal, Canada	Speaker
50	Gutjahr, Johann	University of Duisburg-Essen, Germany	Student
51	Hart, Gus	Brigham Young University, Provo, USA	Speaker
52	Hess, Franziska	University of Marburg, Germany	Student
53	Hofmann, Oliver	Fritz Haber Institute, Berlin, Germany	Postdoc / Tutor
54	Hollmann, Nils	MPI f. Chem. Phys. Solids, Dresden, Germany	Student
55	Isaeva, Leyla	Uppsala University, Sweden	Student
56	Jestaedt, Rene	Fritz Haber Institute, Berlin, Germany	Student
57	Jucha, Anna	University of Wroclaw, Poland	Student
58	Kaliappan, Muthukumar	J.-W. v. Goethe University, Frankfurt, Germany	Postdoc
59	Kavathekar, Ritwik	University College Dublin, Ireland	Student
60	Knuth, Franz	Fritz Haber Institute, Berlin, Germany	Student / Tutor
61	Kraisler, Eli	Weizmann Institute of Science, Rehovot, Israel	Student
62	Kroes, Jaap	EPFL, Lausanne, Switzerland	Student
63	Kurko, Sandra	Institute VINCA, Belgrade, Serbia	Student
64	Lampenscherf, Stefan	Siemens AG, Munich, Germany	Speaker
65	Lazarevic, Florian	Fritz Haber Institute, Berlin, Germany	Student
66	Lepeshkin, Sergey	Russian Academy of Sciences, Moscow	Student
67	Levchenko, Sergey	Fritz Haber Institute, Berlin, Germany	Speaker
68	Liu, Junwei	Tsinghua University, China	Postdoc
69	Liu, Wei	Fritz Haber Institute, Berlin, Germany	Postdoc
70	Lorenzen, Winfried	Universität Rostock, Germany	Student
71	Luo, Hu-Bin	Chinese Academy of Sciences, Shenyang	Student
72	Luo, Ning	Peking University, China	Student
73	Mandal, Subhasish	Michigan Technological University, USA	Student
74	Mangold, Claudia	Fritz Haber Institute, Berlin, Germany	Student / Tutor
75	Marsmann, Martijn	University of Vienna, Austria	Speaker
76	Megow, Jörg	Humboldt University Berlin, Germany	Student
77	Miranda Mena, Joaquin	Forschungszentrum Jülich, Germany	Student
78	Molina-Sanchez, Alejandro	IEMN-CNRS, Villeneuve d'Ascq Cedex, France	Student
79	Moll, Nikolaj	IBM Research, Zurich, Switzerland	Postdoc
80	Morawietz, Tobias	Ruhr-Universität Bochum, Germany	Student
81	Mukhanov, Andrey	Russian Academy of Science, Moscow, Russia	Student
82	Nelson, Lance	Brigham Young University, Provo, USA	Student / Tutor
83	Nemec, Lydia	Fritz Haber Institute, Berlin, Germany	Student / Tutor
84	Ni, Zhenjuan	University of Illinois at Chicago, USA	Student
85	Ortenzi, Luciano	MPI f. Solid State Research, Stuttgart, Germany	Student
86	Palagin, Dennis	Technical University of Munich, Germany	Student
87	Pavlova, Anna	University of Amsterdam, The Netherlands	Student
88	Pilania, Ghanshyam	University of Connecticut, Storrs, USA	Student
89	Pinheiro, Maximiliano	University of Sao Paulo, Brazil	Student
90	Plagemann, Kai-Uwe	Universität Rostock, Germany	Student
91	Pozun, Zachary	University of Texas at Austin, USA	Student
92	Ramirez Caballero, Gustavo	Texas A&M University, USA	Student
93	Rehak, Petr	Brno University of Technology, Czech Republic	Student
94	Ren, Xinguo	Fritz Haber Institute, Berlin, Germany	Speaker
95	Reuter, Karsten	Technical University of Munich, Germany	Speaker
96	Richter, Norina	Fritz Haber Institute, Berlin, Germany	Student
97	Rinke, Patrick	Fritz Haber Institute, Berlin, Germany	Speaker
98	Rizzi, Michele	EPFL, Lausanne, Switzerland	Postdoc
99	Rohr, Daniel	Technical University of Lodz, Poland	Postdoc
100	Rokhmanenkov, Alexander	Russian Academy of Science, Moscow, Russia	Postdoc
101	Rondina, Gustavo	University of Sao Paulo, Brazil	Student

102	Ropo, Matti	Fritz Haber Institute, Berlin, Germany	Postdoc / Tutor
103	Rossi, Mariana	Fritz Haber Institute, Berlin, Germany	Student / Tutor
104	Ruiz López, Victor	Fritz Haber Institute, Berlin, Germany	Student / Tutor
105	Rutckaia, Viktoriia	Phys. Tech. Acad. University, St. Petersburg, Russia	Student
106	Santra, Biswajit	Fritz Haber Institute, Berlin, Germany	Postdoc / Tutor
107	Sauer, Joachim	Humboldt University Berlin, Germany	Speaker
108	Schauer, Volker	Stuttgart University, Germany	Student
109	Scheffler, Matthias	Fritz Haber Institute, Berlin, Germany	Organizer
110	Schmeißer, Martin	Technical University Chemnitz, Germany	Student
111	Schubert, Franziska	Fritz Haber Institute, Berlin, Germany	Student / Tutor
112	Schulthess, Thomas	ETH Zurich, Switzerland	Speaker
113	Scopece, Daniele	University of Milano-Bicocca, Italy	Student
114	Setiawan, Dani	University of Groningen, The Netherlands	Student
115	Shapiro, Joshua	University of California at Los Angeles, USA	Student
116	Si, Chen	Tsinghua University, China	Postdoc
117	Singh, Abishek	FHI-Theory der MPG	Postdoc / Tutor
118	de Melo Souza, Amaury	Trinity College Dublin, Ireland	Student
119	Suleiman, Mohammed	Univeristy of the Witwatersrand, South Africa	Student
120	Tkatchenko, Alexander	Fritz Haber Institute, Berlin, Germany	Speaker
121	Tocci, Gabriele	University College London, England	Student
122	Utecht, Manuel	Potsdam University, Germany	Student
123	Vujasin, Radojka	Vinca Institute of Nuclear Sciences	Student
124	Walkenhorst, Jessica	Universidad del País Vasco, San Sebastian, Spain	Student
125	Walsh, Aron	University College London, England	Speaker
126	Wieferink, Jürgen	Fritz Haber Institute, Berlin, Germany	Speaker
127	Wirth, Jonas	Potsdam University, Germany	Student
128	Wlodarczyk, Radoslaw	Humboldt University Berlin, Germany	Student
129	Xu, Yong	Fritz Haber Institute, Berlin, Germany	Postdoc / Tutor
130	Zhang, Guo-Xu	Fritz Haber Institute, Berlin, Germany	Student / Tutor
131	Zhu, Hong	University of Connecticut, Storrs, USA	Student