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.

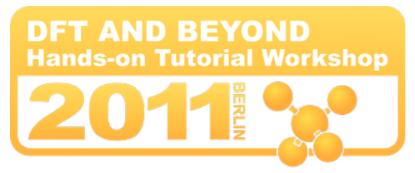
Apart from the discussions and tutorials held at the workshop, the results are available permanently on the world-wide web at:

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, Ju	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, J	uly 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, J	uly 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, Jul	y 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"

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, Ju	ly 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 an	d 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

Density Functional Theory and Beyond 2011 - Participant List

40.0	M 077111 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0 1
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	JW. 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
	•	Student
66 Lepeshkin, Sergey	Russian Academy of Sciences, Moscow	
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
	Technical University of Lodz, Poland	Postdoc
99 Rohr, Daniel 100 Rokhmanenkov, Alexander	Russian Academy of Science, Moscow, Russia	Postdoc
101 Rondina, Gustavo	University of Sao Paulo, Brazil	Student
10 I Nonuma, Gustavo	Oniversity of Gao Faulo, Diazil	Gludeni

Density Functional Theory and Beyond 2011 - Participant List

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