Recent Developments in the Theory Department

Director: Matthias Scheffler

1. General Remarks

From the very beginning, research in the Department has been concerned with fundamental aspects of the *ab initio* thermodynamics and statistical mechanics of surfaces, interfaces, clusters, and nanostructures. Since the last meeting of the *Fachbeirat* more emphasis has been put on *big-data driven science*. The associated concepts and methods belong under the headings: statistical learning, machine learning, data mining, and compressed sensing. This research direction of the *Theory Department* started already 15 years ago with our exploratory work on neural networks. However, only in June 2014 together with Claudia Draxl (Max Planck Fellow at the FHI since July 2014), it was decided to expand the groups' *database on computational materials science results* into a worldwide activity: the *NOMAD (Novel Materials Discovery) Repository*. Together with 8 European scientific groups and 4 European high-performance computer centers this will now be advanced even further, namely to the *NOMAD (European) Center of Excellence (CoE)* which will be inaugurated November 1, 2015. The impact and success of both activities (repository and CoE) is already overwhelming. Details are discussed in Section 4.2 below.

A second vital research direction that we are currently reinforcing is electron-vibrational (or electron-phonon: e-ph) coupling. One important example relates to polarons that may be the charge carriers in certain metal oxides and organic systems. Moreover, the thermoelectric effect is obviously controlled by the e-ph interaction. The above effects are described in terms of corrections to the Born-Oppenheimer (BO) approximation. However, for processes where chemical bonds break and new bonds are formed, i.e. at transition states of chemical reactions, it is possible, if not likely, that the BO approximation breaks down, and new concepts need to be developed.

A third successful development in the Department in recent months has been the continuing work on the description of van der Waals interactions in density functional theory (DFT) calculations. The first paper, published in 2009 (*Accurate Molecular van der Waals Interactions from Ground-State Electron Density and Free-Atom Reference Data, Phys. Rev. Lett.* ***102***), has already attracted more than 1,000 citations, and the methodological improvements since then are remarkable. They will be discussed in the chapter of the ERC (European Research Council) group of Alexandre Tkatchenko.

Finally, but importantly, we mention the *FHI-aims* code. *FHI-aims* is one of the most accurate and numerically most efficient computer codes for extended materials and large and small clus-

ters. The various improvements and advancements, for example, the development of correlation-consistent basis sets for advanced functionals, *GW* approach, and embedding techniques have been highly significant.

A more complete discussion of the breadth of the work of the Department can be found in Sections 4 and 5, and also in the *Yellow Book*, and on the posters displayed in the Department.

The following Section describes organizational developments, and Section 3 addresses personnel and related matters. Subsequently, Sections 4 and 5 briefly outline some of the scientific work performed in the *Theory Department*: Section 4 describes conceptual, methodological, and technical developments, which enable us to study new types of problems and/or to improve the accuracy of calculations. In Section 5, the main applications studied in the *Theory Department* are sketched and some recent results presented.

The presentation focuses on developments of the last 18 months.

2. Organizational

We summarize various aspects of the present situation in bullet form.

- Collaboration with the University of California, Santa Barbara (UCSB, College of Engineering and College of Mathematical, Life, and Physical Sciences) started in 2005. The exchange of postdocs and PhD students between the institutes has turned out to be stimulating and successful. Matthias Scheffler spends about two months per year at the UCSB.
- We are part of an *NSF Partnership for International Research and Education: Electron Chemistry and Catalysis at Interfaces* (PIRE-ECCI). This activity, managed by Susannah Scott at UCSB, helps to intensify collaborations through the exchange of graduate students with chemical-physics institutes in China.
- In 2009 the MPS decided to create *Max Planck Centers* at high-ranking universities outside Germany. The *Theory Department* is part of the *Max Planck - UBC Center for Quantum Materials* which was established in October 2010 at the University of British Columbia (UBC) in Vancouver. The Center is directed by George Sawatzky and Bernhard Keimer who chair a Scientific Board comprised of three Max Planck directors, currently Bernhard Keimer (MPI Stuttgart), Hao Tjeng (MPI Dresden), Matthias Scheffler, and three UBC professors, currently George Sawatzky, Andrea Damascelli, and Ian Affleck.
- At the École Polytechnique Fédérale de Lausanne (EPFL) the *Max Planck - EPFL Center for Molecular Nanoscience and Technology* has been initiated by Klaus Kern (MPI

Stuttgart), together with Benoit Deveaud-Plédran (EPFL), Jeffrey Hubbell (EPFL), Thomas Rizzo (EPFL), Matthias Scheffler, and Alec Wodtke (MPI Göttingen). The official start was January 1, 2013. Several PhD students jointly work with us and colleagues in Lausanne, receiving their PhDs from EPFL.

- In July 2014 Claudia Draxl was appointed *Max Planck Fellow* at the FHI by the President of the MPS. The *Max Planck Fellows* initiative is designed to strengthen the ties between MPIs and universities. Within this framework a small group headed by Claudia Draxl has been set up at the FHI. The work program includes for example studies on hybrid inorganic/organic systems, electron-phonon coupling, thermoelectric materials, and in particular the *NOMAD (Novel Materials Discovery)* project.
- In March 2015 our proposal of a MP partner group on *Advanced Electronic-Structure Methods* at the University of Science and Technology of China (USTC) was granted. It will be led by Xinguo Ren. The objective of the group is to develop advanced and numerically tractable electronic-structure methods to satisfy the increasing needs for higher accuracy and reliability of first-principles calculations in physics and materials science. The official starting date of the group is September 2015, and an inauguration workshop is planned to take place in Hefei in June 2016.
- Every year, the *Fördernde Mitglieder* (*Supporting Members of the MPS)* contribute to a specific project. In 2015 the *NOMAD (Novel Materials Discovery) Repository* was chosen and supported by their donations (details about the *NOMAD* project are described in Section 4.2).
- In October 2014 the *Berlin Big Data Center (BBDC)* was installed. The *BBDC* is a Competence Center funded by the German Ministry of Education and Research (BMBF) which deals with the development of expressive, declarative, fast, and efficient big-data analytics (enabled by Hadoop and Apache Flink), massive-parallel data handling, and more. Matthias Scheffler is one of the 10 principle investigators (PIs), Volker Markl (TU Berlin) is the director of the center.

As of August 1, 2015, the FHI *Theory Department* is structured into 8 research groups. Nevertheless, most of the work in the Department typically involves more than one of these groups. The groups and their leaders are:

- *Unifying Concepts in Catalysis*, headed by **Sergey V. Levchenko**
- *Ab Initio Statistical Mechanics of Cluster Catalysis and Corrosion*, headed by **Luca M. Ghiringhelli**
- *Heat and Charge Transport*, headed by **Matthias Scheffler** (deputy Christian Carbogno)
- *Ab Initio Biomolecular Simulations*, headed by **Carsten Baldauf**
- *Advanced First-Principle Methods for Materials Science and Engineering*, headed by **Igor Ying Zhang**
- *Theoretical Spectroscopy*, headed by **Angel Rubio** (until spring 2016)
- ERC group on *Organic Functional Materials and Molecular Interactions*, headed by **Alexandre Tkatchenko** (see the special chapter for this group)
- *Machine Learning for Materials*, headed by **Matthias Rupp**
- In addition, we host Emeritus **Alexander M. Bradshaw** (since January 2009) who is working on photoionization in molecules and clusters as well as on questions of energy supply and resources in the context of the sustainability debate.

The group headed by Angel Rubio (*Theoretical Spectroscopy*) and the former group of Patrick Rinke (*Many-Body Electronic-Structure Theory*) are gradually moving to the MPI in Hamburg and to the Aalto University in Finland, respectively. However, close collaborations between members of the *Theory Department* and both colleagues will continue in the future. Together with Patrick Rinke, we are working on projects of the Collaborative Research Center (*Sonderforschungsbereich*, SFB) of the German Research Foundation (DFG) on *Hybrid Inorganic/Organic Systems* (HIOS). Angel Rubio is and remains External Scientific Member of the FHI, and he is a PI of the *NOMAD Center of Excellence* (see Section 4.2.2 below).

Together with Martin Vingron (director at the MPI for Molecular Genetics) Matthias Scheffler is responsible for the Joint Network Center (*Gemeinsames Netzwerkzentrum*, GNZ) of the Berlin-Brandenburg Max Planck activities. This is a regional IT competence center, serving 8 MPIs and 6 additional institutions. It focuses on networking, backup, virtualization, and security services. The GNZ is headed by Gerd Schnapka.

3. Personnel and Related Matters

Since the last visit of the *Fachbeirat* in February 2014 the following noteworthy developments have taken place:

- **Matthias Rupp** joined the *Theory Department* in May 2015 as leader of the new group *Machine Learning for Materials*.
- **Igor Ying Zhang** was promoted to group leader in May 2014. His group is called *Advanced First-Principle Methods for Materials Science and Engineering.*
- In September 2014, **Patrick Rinke** became professor at Aalto University in Finland where he started the *Computational Electronic Structure Theory Group* in the Department of Applied Physics. The *Theory Department* continues to collaborate with him on several projects, e.g. within the HIOS-SFB of the German Research Foundation.
- **Saswata Bhattacharya** accepted a position as assistant professor at the Department of Physics at the Indian Institute of Technology Delhi in April 2015. Collaborations with the FHI, in particular with Luca M. Ghiringhelli, continue on machine-learning methods for metal oxide properties and the development of genetic algorithms for cluster-structure global searches.
- February 2015, **Wei Liu** took on a post as professor in the Department of Materials Science and Engineering at Nanjing University of Science and Technology (China).
- **Guo-Xu Zhang** left the FHI in February 2015 to join the Harbin Institute of Technology (China) as lecturer.
- **Alexandre Tkatchenko** recently accepted the offer for the Chair of Theoretical Condensed Matter Physics at the University of Luxembourg. He is planning to move there in November 2015, but will still participate in several ongoing projects at the FHI.

We are also proud to report that three renowned scientists have received prestigious Humboldt Research Awards which support extended research stays at the FHI. In November 2014 **Krishna Rajan** (Iowa State University, USA) received the award for his pioneering work in the emerging field of Materials Informatics. At the same time, **John Perdew** (Temple University, USA) was granted the award for his ground-breaking research on the analysis and development of new XC-functionals for density-functional theory. Both scientists have paid the institute extensive visits this year and are planning to return several times during coming years to

collaborate with scientists of the Department. In April 2015 **Gustavo Scuseria** (Rice University, USA) was awarded the prize for his development, implementation, and application of computational quantum chemistry tools to practical problems.

Mariana Rossi was successfully nominated as Minerva-Fast-Track-Fellow. The program is designed to allow excellent young female scientists a better long-time planning of their career with the aim to increase female scientists in top positions.

Members of the *Theory Department* take part in various national, European (EU and ESF), and international programs. The list of these activities is as follows (sorted alphabetically):

- BMBF – Federal Ministry of Education and Research (Germany), *Berlin Big Data Center (BBDC)*, coordinator: V. Markl; M. Scheffler - since October 2014.
- DFG – German Research Foundation, Cluster of Excellence 314: *Unifying Concepts in Catalysis (UniCat)*, coordinator: M. Driess; M. Scheffler - first funding period: November 2007 - October 2012, new funding period November 2012 - October 2017.
- DFG – German Research Foundation, SFB 951: *Hybrid Inorganic/Organic Systems for Opto-Electronics (HIOS)*, coordinator: N. Koch; project B4: P. Rinke, M. Scheffler; project B10: A. Tkatchenko, M. Scheffler, new funding period: July 2015 - June 2019.
- DFG – German Research Foundation, FOR 1543: *Shear-flow Regulation of Hemostasis (SHENC)*, spokesman: R. Schneppenheim; subgroup C1: F. Gräter, C. Baldauf - first funding period June 2011 - August 2014, new funding period: September 2014 - August 2017.
- Einstein Foundation Berlin – Einstein Research Project *ETERNAL: Exploring Thermoelectric Properties of Novel Materials*, K.-R. Müller, C. Draxl, M. Scheffler - since April 2013.
- EU – European Commission, E-Infrastructures: *NOMAD (Novel Materials Discovery) Center of Excellence*, coordinator: M. Scheffler - starting November 2015.
- Max Planck Society and École Polytechnique Fédérale de Lausanne – *MP-EPFL Center for Molecular Nanoscience and Technology*, directors: K. Kern, T. Rizzo; board members: B. Deveaud-Plédran, J. Hubbel, A. Wodtke, M. Scheffler - since 2013.

  The *Theory Department* is currently involved in three projects of the center: *Biomolecules on Their Way to Solvation*, G. von Helden, C. Baldauf, T. Rizzo (EPFL); *First-Principles*

High-throughput Design and Discovery of Novel Materials, and Its Application to Thermoelectrics, M. Scheffler, N. Marzari (EPFL); *Peptides at Surfaces: Simulating Organic-Inorganic Interface Systems*, M. Ceriotti (EPFL), C. Baldauf, M. Rossi (Oxford University).

- Max Planck Society and University of British Columbia – *MPS-UBC Center for Quantum Materials*, directors: B. Keimer, G. A. Sawatzky; board members: A. Damascelli, L. H. Tjeng, I. Affleck, M. Scheffler - since 2010.
- NSF – The National Science Foundation, Partnership for International Research and Education (PIRE): *Electron Chemistry and Catalysis*, director: S. Scott; M. Scheffler - since 2005.
- UCSB – University of California, Santa Barbara, College of Engineering and College of Mathematical, Life & Physical Sciences; M. Scheffler (distinguished visiting professor for materials science and engineering) - since 2005.
- Vetenskapsrådet – Swedish Research Council: *Catalysis on the Atomic Scale*, organizer: E. Lundgren; S. V. Levchenko, M. Scheffler - since 2011.

We continue our strong involvement and support of CECAM and Psi-k, e.g. by organizing workshops, tutorials, and schools and working in the *CECAM Council* and the *Psi-k Board of Trustees* (the governances of these two organizations).

CECAM is a high-level European organization devoted to the promotion of fundamental research on advanced computational methods and their application to important problems in frontier areas of science and engineering. It is supported by various European research organizations including MPS and DFG. The CECAM headquarters is at the EPFL Lausanne, and *CECAM* nodes have been established in several member states. We are part of the joint node, *cecam-MM1P.de* which focusses on multi-scale modeling from first principles (MM1P) with emphasis on methods and applications to materials and biophysics. The board of directors of the *MM1P.de* node consists of Thomas Frauenheim (University of Bremen), Eberhard K. U. Gross (MPI Halle), Matthias Scheffler, and Björn Winkler (Goethe University Frankfurt). The node will continue to exist at least until 2018.

Psi-k is a Europe-based worldwide network of researchers working on the advancement of first-principles computational materials science. Its mission is to develop fundamental theory, algorithms, and codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form the scientific core. Applications encompass inorganic, organic, and bio-materials

and cover a whole range of diverse scientific, engineering, and industrial endeavors. Key activities of Psi-k are the organization of conferences, workshops, tutorials, and training schools and the dissemination of scientific thinking in society.

Scientists of the *Theory Department* were involved in various services and activities supporting the surface-science and electronic-structure communities worldwide. For example, they lecture at the *Free University Berlin*, the *Technical University Berlin*, and the *Humboldt-Universität zu Berlin* as well as at the *International Max Planck Research School*. They organized or co-organized conferences, workshops, tutorials, and summer schools on topics in electronic-structure theory, multi-scale modeling, surface science, and biophysics, which have impacted upon the careers of very many students of theoretical materials science. The list of activities in the last 18 months includes:

- Symposium on "Frontiers of Electronic Structure Theory: Non-equilibrium Phenomena at the Nano-scale", March 30 - April 4, 2014 at DPG Spring Meeting, Dresden, Germany; organizers: R. Car (Princeton University, USA), K. Sommer Thygesen (Technical University Denmark, Denmark), and M. Scheffler
- Workshop on "White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back", June 16 - 20, 2014, Saint Petersburg, Russia; organizers: E. Blokhin (HU Berlin, Germany), L. M. Ghiringhelli, S. V. Levchenko, and M. Scheffler
- Workshop on "What About *U*? -- Strong Correlations from First Principles", June 17 - 20, 2014, CECAM-HQ-EPFL, Lausanne, Switzerland; organizers: M. Cococcioni (EPFL, Switzerland), S. Biermann (École Polytechnique, Palaiseau Cedex, France), S. de Gironcoli (SISSA and CNR-DEMOCRITOS IOM, Trieste, Italy), and P. Rinke
- An international symposium on "Inorganic Insights into Catalysis" on the occasion of the 60th birthday of Robert Schlögl, July 3 - 4, 2014, Berlin, Germany; organizers: M. Scheffler, A. Trunschke, and J. Pach
- Hands-on summer school on "Density Functional Theory and Beyond: Computational Materials Science for Real Materials", July 21 - August 1, 2014, Los Angeles, USA; organizers: V. Blum (Duke University, USA), C. Carbogno, M. Scheffler, and C. Ratsch (IPAM, USA)
- FHI-aims developers' and users' meeting on "Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals", August 19 - 22, 2014, Berlin, Germany; organizers: V. Blum (Duke University, USA), C. Baldauf, C. Carbogno, and M. Scheffler

- Colloquium on the occasion of the 70th birthday of Alexander M. Bradshaw "Oberflächen, Fusion und mehr", January 30, 2015, Berlin, Germany; organizers: D. Bimberg (TU Berlin, Germany), K. Horn, and M. Scheffler
- CECAM/Psi-k Research Conference on "Frontiers of First-Principles Simulations: Materials Design and Discovery", February 1 - 5, 2015, Berlin, Germany; organizers: G. Ceder (MIT, USA), N. Marzari (EPFL, Switzerland), and M. Scheffler
- Workshop on "Machine Learning for Many-Particle Systems", February 23 - 27, 2015, Los Angeles, California, USA; organizers: A. Aspuru-Guzik (Harvard University, USA), G. Csanyi (University of Cambridge, UK), K.-R. Müller (TU Berlin, Germany), and A. Tkatchenko
- Symposium on "Frontiers of Electronic Structure Theory: Many-body Effects on the Nanoscale", March 15 - 20, 2015 at DPG Spring Meeting, Berlin, Germany; organizers: S. G. Louie (UC Berkeley, USA), E. Runge (TU Ilmenau, Germany), and M. Scheffler
- Workshop on "From Many-Body Hamiltonians to Machine Learning and Back", May 11 - 13, 2015, Berlin, Germany; organizers: A. Tkatchenko and M. Rupp
- Workshop on "Modeling Many-Body Interactions 2015", May 26 - 29, 2015, Castelletto di Brenzone, Italy; organizers: R. A. DiStasio Jr. (Princeton University, USA), A. Ambrosetti (University of Padova, Italy), P. L. Silvestrelli (University of Padova, Italy), and A. Tkatchenko
- Workshop on "Methods and Algorithms in Electronic-Structure Theory", June 3 - 6, 2015, Ringberg Castle, Germany; organizers: M. Kaupp (TU Berlin, Germany), P. Rinke (Aalto University, Finland), P. Saalfrank (University of Potsdam, Germany), and M. Scheffler
- Hands-on workshop on "Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials", July 13 - 23, 2015, Berlin, Germany; organizers: V. Blum (Duke University, USA), C. Baldauf, and M. Scheffler
- Summer School of the Max-Planck-EPFL Center for Molecular Nanoscience & Technology, July 27 - 31, 2015, Ringberg Castle, Germany; organizers: C. Baldauf, C. Carbogno, and M. Scheffler

Alex Bradshaw has served on several committees of the National Academy of Sciences (Leopoldina), National Academy of Engineering (acatech), and the Royal Society in the UK. He is

also a member of an inter-academy study group accompanying the German energy transformation (*Energiewende*) and of the energy steering committee of the European Academies Science Advisory Council (EASAC).

4. New Concepts, Methods, and Techniques

There are two activities which affect, or which are beginning to affect, most of the work in the Department, namely, the continued development of the *FHI-aims code* and the *NOMAD (Novel Materials Discovery)* project. They will be discussed first, followed by more specific issues. The work of the ERC group of Alexandre Tkatchenko will not be described here, but rather in a separate chapter.

4.1 *FHI-aims* Code

The development of the *FHI-aims* code started from an analysis of various electronic-structure theory concepts, in particular the KKR, LMTO, LAPW, and pseudopotential methods. Matthias Scheffler contributed to all of these over the last 40 years or so. In a nutshell, the *FHI-aims* code is as accurate as the best LAPW codes and as fast as *ab initio* pseudopotential codes. At the same time, it is easy to use and designed for massive parallel computers. The code is still "young", but is gaining increasingly in popularity. All developments are coordinated by Volker Blum (Duke University) and Matthias Scheffler. During the last year several advanced functionals have been implemented and significant speed-ups have been achieved for *GW* and RPA (random-phase approximation) calculations. (Xinguo Ren[1], Volker Blum[2], Hermann Lederer[3], Markus Rampp[3], Florian Merz[3], Andreas Marek[3], Christian Carbogno)

Advanced density functionals as well as second order Møller-Plesset perturbation theory (MP2) and coupled-cluster theory (CCSD and CCSD(T)) require particularly sophisticated basis sets. While the development of CCSD(T) for periodic systems is still ongoing, the progress is significant. (Igor Y. Zhang, Tonghao Shen)

[1] University of Science and Technology of China, Hefei, China
[2] Duke University, Durham, USA
[3] Max Planck Computing and Data Facility, Garching, Germany

4.2 *NOMAD (Novel Materials Discovery)* Project

The *NOMAD* project started in 2012 as a joint group activity of Claudia Draxl and Matthias Scheffler funded by the Einstein Foundation. In June 2014 it was decided, to extend it into *i)* a world-wide operating repository for input and output files of *ab initio* electronic structure codes and to seek funding within HORIZON 2020 for *ii)* a Center of Excellence (together with 12 other European partners). Having been recently granted, a code-independent data base will soon be developed that in turn will be complemented by an extensive *Materials Encyclopedia*, graphics, and a big-data analytics environment.

4.2.1 *NOMAD Open Access Repository*

The *NOMAD open access repository* was established to host, organize, and share materials data. It enables the confirmatory analysis of computational materials data, their re-use, and re-purposing for applications not corresponding to the intention of the original calculations and publications. Uploading of data is possible without any barriers, i.e. results are accepted in their raw format as produced by the underlying code. The only conditions are that the list of authors is provided, and that code and code versions can be retrieved from the uploaded files. For a period up to three years, access to these data can be restricted to the owner or made available to other people (selected by the owner). The "open access" data can be downloaded by any user without even registering.

A summary of the concept and a basic tutorial can be found on YouTube:

concept: https://www.youtube.com/watch?v=L-nmRSH4NQM

tutorial: https://www.youtube.com/watch?v=5Xfzj-degqc

Since February 2015 already several hundred thousand files have been uploaded. Presently 10 different electronic-structure codes are supported. (Luca M. Ghiringhelli, Fawzi R. Mohamed, Lorenzo Pardini[4], Christian Carbogno, Claudia Draxl[4])

4.2.2 *NOMAD-Laboratory, a European Center of Excellence (CoE)*

The *NOMAD CoE* is funded by the European Commission in its E-Infrastructures program. It is a joint activity of 8 scientific groups and 4 high-performance computer centers in Europe. The PIs are: A. Bode (Leibniz-Rechenzentrum, Garching), C. Draxl (HU Berlin), D. Frenkel (University Cambridge), S. Heinzel (MPS Data and Computing Facility), F. Illas (University

[4] Humboldt-Universität zu Berlin, Germany

of Barcelona), K. Koski (CSC-IT Center for Scientific Computing, Helsinki), J. M. Cela (Barcelona Supercomputing Center), R. Nieminen (Aalto University), A. Rubio (MPI MPSD, Hamburg), M. Scheffler, K. Thygesen (Technical University Denmark, Lyngby), A. De Vita (King's College London). The starting date is November 1, 2015.

The main goals are to build a materials encyclopedia and to develop new tools for big-data analytics. However, for the next 12 months the first big challenge will be to build a code-independent data base, accepting the results from about 40 different electronic-structure codes, with the *NOMAD Repository* as a starting point. Force-field studies will be included as well. (Luca M. Ghiringhelli, Fawzi R. Mohamed, Christian Carbogno, Claudia Draxl[4])

4.3 Validation and Verification of Codes, Basis Sets, and XC-Functionals

Validation and verification of codes, basis sets, XC-functionals, treatment of relativity, and pseudopotentials (if used) have been very much neglected in computational materials science. The same holds for the question about the accuracy and error bars of the various approximate functionals that describe the many-electron exchange and correlation (XC). Recently, we have begun to address this weakness; the corresponding activities are briefly summarized below.

4.3.1 Equation of State for Elemental Solids and PBE XC

The *ab initio* materials science community is dealing with many different codes. K. Lejaeghere and S. Cottenier from Gent University, Belgium, initiated a community effort addressing the question: "do two different DFT codes or pseudopotentials really yield identical predictions?". For this, 15 different codes were compared with respect to the calculated equations of state for 71 elemental crystals. The *FHI-aims* code was part of this study. The best three codes, WIEN2k, exciting, and *FHI-aims* have the same quality. CPU-time requirements and user-friendliness were not part of the analysis, but in these issues the *FHI-aims* code shows the best performance. (Volker Blum[2], Alexandre Tkatchenko, Guo-Xu Zhang)

4.3.2 Test Set for Materials Science and Engineering

A test set for materials science and engineering (MSE) is at present being established with well-converged theoretical reference values for a hierarchy of methods, from (semi-)local density-functional approximations (DFAs) to the state-of-the-art MP2 and RPA, thus setting the standard for the implementation and applicability of electronic-structure methods for solids. At this

point, the MSE test set contains results for first and second row elements and their binary compounds with various cubic crystal structures and bonding characters, allowing for systematic benchmarking of manifold chemical interactions. (Igor Y. Zhang, Norina Richter, Xiangyue Liu, Sergey V. Levchenko, Luca M. Ghiringhelli)

4.3.3 *GW*100: Benchmarking G_0W_0 for Molecular Systems

We established a benchmark set of 100 molecules that comprises well-converged ionization potentials and electron affinities computed at the G_0W_0@PBE level. Experimental values are included for reference. While benchmarking electronic-structure methods and implementations have become standard practice in quantum chemistry, we have for the first time benchmarked three *GW* codes. We found unprecedented agreement between the local-orbital codes TURBOMOLE and *FHI-aims* and good agreement with the plane-wave code BerkeleyGW. We expect that the *GW*100 test set will be a cornerstone in future methods development for excited states. (Patrick Rinke[5], Xinguo Ren[1])

4.4 Electron-Phonon Coupling and Heat Transport

Electron-phonon (e-ph) coupling causes a noticeable renormalization of bandgaps in semi-conductors and of charge carriers (formation of polarons). We analyzed the strong sensitivity of e-ph matrix elements on the choice of the approximate XC functionals in DFT. Indeed, the use of hybrid functionals is mandatory, and the parameter α that determines the amount of exact exchange, may be chosen to minimize the localization/delocalization error. The latter is also called the "piecewise linear condition" and represents a property of exact DFT. (Sebastian Kokott, Honghui Shang, Christian Carbogno, Sergey V. Levchenko, and Patrick Rinke[5])

The accurate assessment of heat transport in materials with large thermal conductivity is computationally extremely challenging with *ab initio* molecular dynamics, since the strong harmonic character of the interatomic interactions typically leads to long phonon lifetimes and mean free paths. To overcome this hurdle, we have implemented a transformation formalism that translates between real space trajectories and occupations in reciprocal phonon space, which enables to apply reliable inter- and extrapolation techniques. In turn, this reduces the required computational effort by four orders of magnitude, as we demonstrate for silicon both for semi-empirical potentials and within an *ab initio* framework. (Christian Carbogno)

[5] FHI and Aalto University, Finland

4.5 Towards a Density-Functional Theory for Quantum Electrodynamics (QEDFT)

In order to construct a QEDFT we employ the Sham-Schlüter equation as this provides a direct way to connect the nonlocal self-energy of many-body perturbation theory with the local effective Kohn-Sham potential of QEDFT. In this way, the static as well as the time-dependent optimized effective potential (OEP) integral equations are derived for QED that takes the coupling of quantized electrons and photons into account. (Johannes Flick, Christian Schäfer[6], Camilla Pellegrini[7], Heiko Appel, Michael Ruggenthaler[6], Ilya V. Tokatly[8], Angel Rubio[9])

4.6 Density Functionals Applied to Molecular Dissociation

Starting from the Bethe-Goldstone equation (BGE) which provides the exact solution of one- and two-electron systems, we propose a non-empirical screened second-order BGE (sBGE2) correlation functional with a simplicity comparable to standard second-order perturbation theory. In conjunction with the exact exchange, the sBGE2 approximation provides an accurate description of both H_2^+ and H_2 dissociations, which so far was a big challenge in DFAs. We also extend sBGE2 to a general-purpose orbital-dependent functional, which provides a satisfactory description of N_2 and C_2 dissociations, which is a challenge for DFT as well as for wave-function theory. More importantly, this difficult challenge is conquered together with a consistent improvement over (semi)-local density functionals for various chemical situations, including atomization energies, reaction barriers, and weak interaction. (Igor Y. Zhang, Patrick Rinke[5])

5. Applications – Some Highlights

This Section briefly sketches some application highlights and certain results and insights obtained during the last one and a half years. Not all of this work has been published or submitted for publication. Work predominantly done in Alexandre Tkatchenko's ERC group is discussed in his chapter.

[6] MPI for the Structure and Dynamics of Matter, Hamburg, Germany
[7] Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain
[8] IKERBASQUE, Basque Foundation for Science, Bilbao, Spain
[9] FHI and MPI for the Structure and Dynamics of Matter, Hamburg, Germany

5.1 Surfaces, Adsorption, and Heterogeneous Catalysis

5.1.1 Graphene on 3C-SiC and H Intercalation

Graphene can be grown on various substrates, among which silicon carbide (SiC) supports some of the highest-quality films. Using the *ab initio* atomistic thermodynamics approach, we had previously studied graphene films at the Si-terminated side of 3C-SiC(111). In recent months we extended this work to the C-terminated 3C-SiC(111) surface, considering many possible structures and Si and C reservoirs at any reasonable temperature and pressure. We identified a hitherto unknown lowest-energy (3×3) graphene precursor structure in excellent agreement with experimental STM images. In general, we find that graphene will only be stable when the SiC substrate is becoming unstable which makes monolayer graphene growth on the C-side of SiC very difficult. (Lydia Nemec, Patrick Rinke[5], Jan Kloppenburg[10], Björn Lange[2], Volker Blum[2])

5.1.2 *Ab initio* Atomistic Thermodynamics for Various Adsorbate Systems: Adsorbate Phases, Clustering, and Coverage-Dependent Chemistry

Two different classes of systems were considered: *a)* H_2O at *M*O (001), with *M* = Ca, Mg, Sr and *b)* H and CH_x at Ru (0001) with x = 0-4. For the XC treatment, we used the PBE and HSE06 hybrid functional combined with the self-consistent many-body dispersion approach. The structure search was performed using a first-principles genetic algorithm.

For *a)*, the results predict ordered one-dimensional (1D) adsorbed water structures on CaO(001), which is in agreement with scanning tunneling microscopy and infrared spectroscopy studies performed in the CP Department. On MgO(001) and SrO(001) such water structures are not found to be stable. CaO(001) is special and only here the proper balance between adsorbate-adsorbate and adsorbate-surface interactions is reached, which is largely ruled by the substrate lattice constant.

Part *b)* of this work is a collaboration with the PC Department. Here, the influence of hydrogen adsorption on the adsorption and reactions of CH_x (x = 0-4) on Ru(0001) is studied at realistic temperatures and hydrogen pressures. Adsorbed hydrogen changes the preferred site and the stability of CH_2 species, which is crucial for understanding the Fischer-Tropsch synthesis. Moreover, adsorbed hydrogen is found to have a profound influence on the C-C coupling reactions: While it generally reduces all the coupling reaction barriers, some reaction pathways become more favorable. (Xunhua Zhao, Sergey V. Levchenko)

[10] FHI and Duke University, Durham, USA

5.1.3 Effects of Surface-Site Coordination on the Thermodynamic Stability of Point Defects

We analyzed the thermodynamic stability of O-vacancy and O/O_2-ad-species at steps and corners at MgO surface. The defects are modelled using MgO clusters, described at the hybrid-functional level and embedded into a field of norm-conserving non-local pseudopotentials and point charges. The low-energy defect structures are found using an *ab initio* genetic algorithm. The long-range response of the oxide to the charge carriers trapped at the defects is taken into account using a polarizable force field. Unexpectedly, we found that O-ad-species rather than O-vacancies are the dominant defects at realistic conditions. This is explained by an interplay between bond-breaking, bond-making, and charge-carrier trapping. (Saswata Bhattacharya[11], Daniel Berger[12], Karsten Reuter[12], Sergey V. Levchenko, Luca M. Ghiringhelli)

5.2 Organic Materials and Interfaces

5.2.1 Length Dependence of Ionization Potentials of Trans-Acetylenes Studied by an Internally Consistent DFT/*GW* Approach

The Ionization Potential (IP) was calculated for the paradigmatic quasi-one-dimensional trans-acetylene family of conjugated molecules, from short to long oligomers and to the infinite polymer trans-polyacetylene (TPA). Our IP predictions are based on an "internally-consistent" scheme: We adjust the exchange mixing parameter α of the PBEh hybrid density functional, so that the highest-occupied Kohn-Sham level of DFT-PBEh(α*) agrees with the IP calculated from *GW*@PBEh(α*). We find that α* is system-dependent and converges with increasing oligomer length. Also the IP varies with oligomer length, and it converges to the value for TPA with a smooth, inverse-length-exponential behavior. (Maximilian Pinheiro Jr.[13], Marilia J. Caldas[13], Patrick Rinke[5], Volker Blum[2])

5.2.2 Integer versus Fractional Charge Transfer at Metal(/Insulator)/Organic Interfaces: Cu/TCNE and Cu/NaCl/TCNE

Semilocal and hybrid density-functional theory was used to study the charge transfer and the energy-level alignment at a representative interface between an extended metal substrate and an organic adsorbate layer. Upon suppressing electronic coupling between the adsorbate and the substrate by inserting thin, insulating layers of NaCl, the hybrid functional localizes electronic charge. The laterally inhomogeneous charge distribution resulting from this spontaneous

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[12] Technische Universität München, Germany
[13] Universidade de São Paulo, Brasil

breaking of translational symmetry is reflected in observables such as the molecular geometry, the valence and core-level spectroscopy, and the evolution of the work function with molecular coverage.

The studies were extended to the adsorption of organic molecules on the wide-bandgap, *n*-doped ZnO. Here, the molecules exhibit a combination of charge transfer and backtransfer, reminiscent of the Blyholder model of CO adsorption. (Oliver T. Hofmann[14], Patrick Rinke[5], Georg Heimel[4])

5.2.3 Pressure Dependence of Band Parameters of Organic Semiconductors

Band gaps, effective masses, and electric conductivities of semiconductors noticeably depend on strain that may be imposed by fabrication conditions of practical devices. Previously, we had studied these issues for inorganic semiconductors. Now we have investigated two prototypical organic systems, namely trans-polyacetylene and anthracene. For these materials, the state-of-the-art density-functional approximations do not provide a reliable description.

The calculations reveal that the electronic band structure and gap of crystalline trans-polyacetylene are not only determined by the dimerization, but are also influenced by interchain interactions, which lead to a splitting of valence and conduction band. Corresponding results are found for crystalline anthracene. We also computed the pressure-dependent electronic transport coefficients for both organic semiconductors using the Boltzmann transport equation in the constant relaxation time approximation. (Franz Knuth, Christian Carbogno, Volker Blum[2])

5.2.4 Insight into Organic Reactions from the Random-Phase Approximation and its Corrections

The performance of the random-phase approximation (RPA) and beyond-RPA approximations for the treatment of electron correlation are benchmarked on three different molecular test sets. The test sets are chosen to represent three typical sources of error which can contribute to the failure of most density-functional approximations in chemical reactions. The first test set (atomization and n-homodesmotic reactions) offers a gradually increasing balance of error from the chemical environment. The second test set (Diels-Alder reactions cycloaddition = DARC) reflects more the effect of weak dispersion interactions in chemical reactions. Finally, the third test set (self-interaction error 11 = SIE11) represents reactions which are exposed to noticeable

[14] Graz University, Austria

self-interaction errors. This work seeks to answer whether a universal many-body approximation exists to address all these challenges. (Adrienn Ruzsinszky[15], Igor Y. Zhang)

5.3 Biophysics

5.3.1 Improving the Theoretical Description of Peptide-Cation Interactions

Metal cations trigger the three-dimensional structure of peptides and proteins, but can also cause misfolding as it is discussed, for example, in Alzheimer's disease. The understanding of the atomistic basis of the effect of metal cations requires a reliable description of the energetics. Based on representative amino acid-cation complexes, we assessed the accuracy of energy functions in comparison to coupled-cluster theory. Empirical force fields (FF) severely fail to reproduce the reference data, mainly due to the static assignment of partial charges in conventional FF. Density-functional approximations offer higher accuracy, but the often-stressed "chemical accuracy" is only reached with hybrid functionals augmented by a dispersion correction. (Markus Schneider[16], Volker Blum[2], Carsten Baldauf)

5.3.2 Sampling and Representing the Potential-Energy Surface of Molecules from First Principles

The frequent inadequacy of empirical FF to correctly describe the structures and energetics of bio-organic molecules motivated us to develop the software *Fafoom* that performs structure searches using the all-electron code *FHI-aims*. The result of such search is an ensemble of low-energy minima. The relative location of these minima to each other is described by means of their distance in torsion-angle space. Applying a sensible cut-off to long distances allows for drawing a network with nodes being the minima and edges being the distance between them. This identifies a set of likely direct transitions on which we employ transition state searches with the *aimsChain* routine (by Luca M. Ghiringhelli and Yingyu Yao[17]). The collected information, i.e. energies of minima and transition states, represents a reduced potential-energy surface that can be illustrated as barrier tree or disconnectivity graph. (Adriana Supady, Volker Blum[2], Carsten Baldauf)

[15] Temple University, Philadelphia, USA
[16] FHI and MP – EPFL Center, Lausanne, Switzerland
[17] FHI and UBC-MPS Center, Vancouver, Canada

5.3.3 Protein-Ligand Interactions from Semi-Empirical Quantum Mechanics

The current standard in describing the interaction between small molecular ligands and large biological macromolecules (proteins) are empirical energy functions that are trained to reproduce static crystal-structure data. However the complicatedness of the involved interactions (e.g. charge transfer, van der Waals, H bonding) is not described reliably by commonly used simplified functional forms. We demonstrate that a combination of the semi-empirical PM6 method (augmented with corrections for H bonding, dispersion, and halogen bonds) in conjunction with the implicit solvent model COSMO performs superior to the standard methods in describing structure and energetics of the binding-energy landscape of protein-ligand interactions. (Adam Pecina[18], René Meier[19], Pavel Hobza[18], Carsten Baldauf)

5.4 And more…

5.4.1 Thermoelectric Materials

In order to convert some of the significant amount of waste heat into electricity, a better understanding of electron-phonon coupling and heat transport is required (see Section 4.4). Clathrates and skutterudites have been identified as particularly promising materials for thermoelectric applications and both materials classes are presently studied in the Department in collaboration with Claudia Draxl[4] and the experimental group of Juri Grin[20]. In collaboration with them we discuss the implications of our theoretical findings for the synthesis of novel thermoelectric materials with improved heat-transport properties.

For Si_{46} and Ge_{46} clathrates, we find fundamentally different distortions and stabilities of the vacancy, in spite of the isoelectronicity of these two materials. Consequently, these two materials also behave differently upon filling their cages with K or Ba. For Ge-based clathrates, K or Ba guest atoms favor the formation of 2 or 3 vacancies, □, and the lowest free-energy structures (including vibrational and configurational entropies) are $K_8Ge_{44}□_2$ and $Ba_8Ge_{43}□_3$. Conversely vacancy formation is energetically unfavorable in filled Si_{46} clathrates. These results resolve some experimental dubieties.

Using a cluster-expansion of DFT total energies, we have extended these investigations to ternary clathrates such as $(Sr, Ba)_8Al_xSi_{46-x}$.

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[19] Universität Leipzig, Germany
[20] MPI for Chemical Physics of Solids, Dresden, Germany

For $CoSb_3$ and $CoAs_3$ skutterudites, we are presently performing a systematic analysis of the vibrational properties as function of the filling with guests (Ga, In, Sn, etc.). It is found that different guests exhibit very different vibrational dynamics ranging from coherent phonon modes to the formation of localized polarons. (Amrita Bhattacharya, Susmita Basak, Maria Troppenz[4], Santiago Rigamonti[4], Christian Carbogno, Claudia Draxl[4])

5.4.2 Quantum Electrodynamics

For the case of density-functional theory for quantum electrodynamics, we have so far considered prototypical model systems that are commonly used in quantum optics, as well as one-dimensional real-space models. Our results for these systems are very promising and we are currently working on an implementation of our approach for real systems. (Johannes Flick, Christian Schäfer[6], Camilla Pellegrini[7], Heiko Appel, Michael Ruggenthaler[6], Ilya V. Tokatly[8], Angel Rubio[9])

5.4.3 Big-Data Driven Materials Science; Importance of Causal Descriptors

Machine learning is able to identify structure in big data that may be invisible to humans. We have emphasized and demonstrated that successful learning should be based on a set of descriptive, physically meaningful parameters (termed descriptors) that are related to the property of interest. Employing compressed sensing strategies that had been originally developed and used in the field of signal processing, we are able to identify the optimum descriptors. Applications to quantitative structure identification of crystals and to bandgaps of semiconductors demonstrate the importance of causal descriptors. For example, even when carbon containing materials are not included in the learning process, the approach predicts the existence and extraordinary high stability of C-diamond. (Luca M. Ghiringhelli, Sergey V. Levchenko, Claudia Draxl[4])

5.4.4 Machine Learning of Quantum Mechanical Properties of MgO Clusters

Electronic-structure calculations of similar systems contain redundant information. Machine learning (ML) models exploit this to interpolate between a computationally feasible number of *ab initio* reference calculations possibly enabling computational savings of several orders of magnitude. For a diverse set of 9,000 small organic molecules Matthias Rupp has developed a ML model to predict proton and carbon nuclear magnetic resonance chemical shifts, core level excitations, and forces on atoms, reaching accuracies close to the underlying DFT reference data. Metal-oxide clusters are more challenging due to their larger flexibility of bonding. First

results indicate that these ML models can be trained on such systems as well, estimating Mulliken and Hirshfeld partial charges in a dataset of 3,000 MgO clusters with a relative root mean squared error of 2.1-3.1%. (Matthias Rupp, Saswata Bhattacharya[11], Luca M. Ghiringhelli)

5.4.5 Risks, Resources, and Resilience

Several times in the last few decades the possibility of raw material scarcity, even of raw material exhaustion, has given rise to concern. Prominent catchwords in this debate have been, for example, "oil crisis", "geo-political factors", "resource security", "rare earth elements", and "mineral depletion". It transpires that immediate concern is largely unwarranted, although our society does well to think about the sustainable stewardship of natural resources, as well as the search for resilient solutions. In any case, it is legitimate to ask whether supply risk can be assessed and put on a semi-quantitative, comparative basis – not an easy task in an area containing so many socio-economic concepts. Using appropriate indicators we present here a comparative study of the supply risks associated with the constituent elements in two types of thin film photovoltaic module, CdTe, and CIGS. On the basis of the indicators used (geochemical parameters, market data, political assessment indices, etc.) and their weighting using an analytical hierarchy process, CdTe modules are found to be marginally more secure from a supply risk perspective. (Alexander M. Bradshaw, Christoph Helbig[21], Christoph Kolotzek[21], Andrea Thorenz[21], Axel Tuma[21])

[21] University Augsburg, Germany

6. Publications of the Theory Department[22]

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[22] OPEN ACCESS = Gold open access publication

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Doctoral Thesis

Schubert, F.: Conformational equilibria and spectroscopy of gas-phase homologous peptides from first principles. Freie Universität Berlin 2014.

Zhang, G.-X.: Understanding the role of van der Waals forces in solids from first principles. Freie Universität Berlin 2014.

2015

Aponte-Santamaría, C., V. Huck, S. Posch, A.K. Bronowska, S. Grässle, M.A. Brehm, T. Obser, R. Schneppenheim, P. Hinterdorfer, S.W. Schneider, C. Baldauf and F. Gräter: Force-Sensitive Autoinhibition of the von Willebrand Factor ls Mediated by Interdomain Interactions. Biophysical Journal **108** (9), 2312-2321 (2015).

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Gao, W. and A. Tkatchenko: Sliding Mechanisms in Multilayered Hexagonal Boron Nitride and Graphene: The Effects of Directionality, Thickness, and Sliding Constraints. Physical Review Letters **114** (09), 096101 (2015).

Ghiringhelli, L.M. and S.V. Levchenko: Strengthening gold-gold bonds by complexing gold clusters with noble gases. Inorganic Chemistry Communications **55**, 153-156 (2015).

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Rupp, M.: Special issue on machine learning and quantum mechanics. International Journal of Quantum Chemistry **115** (16), 1003-1004 (2015).

Schubert, F., K. Pagel, M. Rossi, S. Warnke, M. Salwiczek, B. Koksch, G.von Helden, V. Blum, C. Baldauf and M. Scheffler: Native like helices in a specially designed β peptide in the gas

phase. Physical Chemistry Chemical Physics **17** (7), 5376-5385 (2015).

Schubert, F., M. Rossi, C. Baldauf, K. Pagel, S. Warnke, G. von Helden, F. Filsinger, P. Kupser, G. Meijer, M. Salwiczek, B. Koksch, M. Scheffler and V. Blum: Exploring the conformational preferences of 20-residue peptides in isolation: Ac-Ala_{19}-Lys + H^+ vs. Ac-Lys-Ala_{19} + H^+ and the current reach of DFT. Physical Chemistry Chemical Physics **17** (11), 7373-7385 (2015).

Sezen, H., H. Shang, F. Bebensee, C. Yang, M. Buchholz, A. Nefedov, S. Heissler, C. Carbogno, M. Scheffler, P. Rinke and C. Wöll: Evidence for photogenerated intermediate hole polarons in ZnO. Nature Communications **6** (4), 6901 (2015).

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Sinai, O., O.T. Hofmann, P. Rinke, M. Scheffler, G. Heimel and L. Kronik: Multiscale approach to the electronic structure of doped semiconductor surfaces. Physical Review B **91** (7), 075311 (2015).

Tkatchenko, A.: Current Understanding of Van der Waals Effects in Realistic Materials. Advanced Functional Materials **25** (13), 2054-2061 (2015).

Zhao, X., X. Shao, Y. Fujimori, S. Bhattacharya, L.M. Ghiringhelli, H.-J. Freund, M. Sterrer, N. Nilius and S.V. Levchenko: Formation of Water Chains on CaO(001): What Drives the 1D Growth? The Journal of Physical Chemistry Letters **6** (7), 1204-1208 (2015).

Doctoral Thesis

Nemec, L.: Graphene Engineering: An *ab initio* Study of the Thermodynamic Stability of Epitaxial Graphene and the Surface Reconstructions of Silicon Carbide. Humboldt-Universität zu Berlin 2015.

7. Invited Talks of the Members of the Theory Department

Guillem Albareda Piquer

Jan 2014 — 6th International Workshop and School on Time-Dependent Density-Functional Theory: Prospects and Applications, Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spain
Non-Adiabatic Dynamics with the Conditional Wave Functions

May 2014 — CECAM Workshop, Recent progress in adiabatic and non-adiabatic methods in quantum dynamics, Lausanne, Switzerland
A Correlated Electron-Nuclear Dynamics with Conditional Wave Functions

Heiko Appel

Jan 2014 — 6th International Workshop and School on Time-Dependent Density-Functional Theory: Prospects and Applications, Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spain
Real-Time Evolution of Correlated Photon-Electron Wavefunctions in Quantum Electrodynamics

Apr 2014 — Block Course, International Max Planck Research School Functional Interfaces in Physics and Chemistry, Berlin, Germany
Introduction to Static and Time-Dependent Density-Functional Theory

Jun 2014 — International Workshop, White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back, St. Petersburg, Russia
Rieman-Silberstein Vector and Photon Wavefunctions in Quantum Electrodynamics

Jun 2014 — Seminar, Faculty of Physics, Bielefeld University, Bielefeld, Germany
Density Functional Theory for Quantum Electrodynamics: Bridging Quantum Optics and Electronic Structure Theory

Dec 2014 — Seminar, Institute of Physics, University of Rostock, Rostock, Germany
Fock Space Evolution and Electron-Photon Correlations in Quantum Electrodynamics

Carsten Baldauf

May 2014 — FHI-Workshop on Current Research Topics at the FHI, Potsdam, Germany
Peptide Secondary Structure Formation in the Gas Phase from First Principles

Aug 2014 — FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany
Structure and Dynamics of Peptide Foldamers from First Principles

Oct 2014 — Seminar, Institute of Pharmacy, Freie Universität Berlin, Berlin, Germany
Mechano-Reception in the A Domains Regulates VWF Structure and Function

Nov 2014 — Dagstuhl Seminar, Algorithmic Cheminformatics, Dagstuhl, Germany
Conformational Search and Landscape Representation for Peptide Foldamers

Feb 2015	XVII. Annual Linz Winter Workshop, Advances in Single-Molecule Research for Biology & Nanoscience, Linz, Austria *Structure and Dynamics of Peptide Foldamers from First Principles*
Mar 2015	1st Ion Mobility-Mass Spectrometry Workshop, FHI, Berlin, Germany *Calculating Theoretical CCSs*
Jul 2015	Summer School of the Max Planck-EPFL Center for Molecular Nanoscience and Technology, Schloss Ringberg, Kreuth, Germany *MD, Vibrational Spectroscopy*
Sep 2015	Psi-k 2015 Conference, San Sebastian, Spain *Methods to Study and Represent the Potential-Energy Surface (PES) of Biomolecules in Isolation*

Björn Bieniek

Jun 2014	International Workshop, White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back, St. Petersburg, Russia *Ultra-Thin ZnO on Metal Substrates: Electronic Structure and Thermodynamic Stability*
Aug 2014	FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany *HDF5 and ESP-Charges in FHI-aims*

Volker Blum

Dec 2013	2013 Fall MRS Meeting and Exhibit, Materials Research Society, Boston, MA, USA *An Integrated All-Electron Path to Theory-Driven Materials Development*

Christian Carbogno

Nov 2013	IPAM Program, Materials for a Sustainable Energy Future, Workshop IV: Energy Conservation and Waste Heat Recovery, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *High Temperature Thermal Conductivity from First Principles*
Apr 2014	Team Meeting on ETSF Electron-Phonon Coupling, Zeuthen, Germany *High Temperature Thermal Conductivity from First Principles*
Jun 2014	International Workshop, White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back, St. Petersburg, Russia *High Temperature Thermal Conductivity from First Principles*
Jul 2014	IPAM Workshop, Density Functional Theory and Beyond: Computational Materials Science for Real Materials, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Thermal Transport in Solids from First Principles*
Aug 2014	FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany *Thermal Conductivity Simulations: Achieving Time and Size Convergence*

Aug 2014	Hands-on Workshop on Excitations in Solids 2014, HoW exciting! Humboldt-Universität zu Berlin, Berlin, Germany *Thermal Conductivity*
Sep 2014	EUPHONON Workshop, Building a European NanoPhononics Community, Le Mans, France *Thermal Conductivities at High Temperatures from First Principles*
Oct 2014	3rd Science Day of the Max Planck-EPFL Center for Molecular Nanoscience and Technology, Berlin, Germany *Towards the First-Principles Discovery of (Novel) Thermoelectric Materials*
Dec 2014	Gruppenseminar, Institute of Theoretical Chemistry, Ulm University, Ulm, Germany *Towards the First-Principles Discovery of (Novel) Thermoelectric Materials*
Jan 2015	Team Meeting on ETSF Electron-Phonon Coupling, Rome, Italy *Thermal Conductivity Simulations: Achieving Time and Size Convergence*
Jan 2015	Winter Workshop, Frontiers of Multiscale Modelling - Current Obstacles and New Horizons for Energy, Materials, and Catalysis, Stubachtal, Austria *Thermal Conductivity Simulations: Reaching the Meso- and Macroscale*
Mar 2015	APS March Meeting 2015, American Physical Society, San Antonio, TX, USA *Accurate Thermal Conductivities from First Principles*
Apr 2015	Kolloquium des Graduiertenkollegs, University of Rostock, Rostock, Germany *Accurate Thermal Conductivities from First Principles*
May 2015	FHI-Workshop on Current Research Topics at the FHI, Potsdam, Germany *Heat Transport from First Principles*
Jun 2015	CECAM Workshop, Future Technologies in Automated Atomistic Simulations, Lausanne, Switzerland *Challenges in Novel Materials Discovery (NOMAD) Using Big Data Paradigms*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Phonons, Electron-Phonon Coupling and Transport in Solids*
Jul 2015	Summer School of the Max Planck-EPFL Center for Molecular Nanoscience and Technology, Schloss Ringberg, Kreuth, Germany *Thermal Conductivities from First Principles Molecular Dynamics*

Luca M. Ghiringhelli

Jun 2014	International Workshop, White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back, St. Petersburg, Russia *Big Data of Materials Science: Critical Role of the Descriptor*
Aug 2014	IPAM Workshop, Density Functional Theory and Beyond: Computational Materials Science for Real Materials, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Search for Minimum Energy Paths: Nudged Elastic Band and Beyond*

Aug 2014	IPAM Workshop, Density Functional Theory and Beyond: Computational Materials Science for Real Materials, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Statistical Mechanics and Molecular Dynamics*
Aug 2014	XXVI IUPAP Conference on Computational Physics, CCP2014, Boston, MA, USA *Big Data of Materials Science – Critical Role of the Descriptor*
Oct 2014	Hands-on Course, International Max Planck Research School (IMPRS), Berlin, Germany *Ab initio Statistical Mechanics of Surfaces, Defects and Clusters*
Dec 2014	AScI Workshop, Machine Learning for Materials Science, Aalto University, Helsinki, Finland *Big Data of Materials Science: Critical Role of the Descriptor*
Dec 2014	Workshop on Simulation and Modeling of Emerging Electronics 2014, University of Hong Kong, Hong Kong, China *Big Data of Materials Science: Critical Role of the Descriptor*
Feb 2015	CECAM Conference, Frontiers of first-principles simulations: materials design and discovery, Berlin, Germany *(Statistical) Learning from (Big) Data in Materials Science: The Critical Role of the Descriptor*
Apr 2015	CECAM Workshop, Emergent structural and electronic phenomena at interfaces of nanoscale oxides, Lausanne, Switzerland *Theoretical Evidence of Unexpected O-Rich Phases in MgO Clusters and at Corners of Extended MgO Surfaces*
May 2015	CECAM/Psi-k Workshop, From Many-Body Hamiltonians to Machine Learning and Back, Berlin, Germany *Design of the Feature Space for Feature-Selection Algorithms Yielding Physically Interpretable Descriptors*
May 2015	FHI-Workshop on Current Research Topics at the FHI, Potsdam, Germany *Learning Physically Meaningful Descriptors from Data in Materials Science*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Ab initio Molecular Dynamics and Nuclear Quantum Effect*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Big-Data Analytics in Materials Science*
Sep 2015	Psi-k 2015 Conference, San Sebastian, Spain *Big Data of Materials Science: Critical Next Steps*

Arvid Ihrig

Aug 2014	FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany *Localized Resolution of Identity: Accurate and Efficient Evaluation of the Coulomb Operator for Advanced Electronic Structure Methods*

Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Local RI, Correlation and Low-Scaling Hybrids*

Sergey V. Levchenko

May 2014	FHI-Workshop on Current Research Topics at the FHI, Potsdam, Germany *Effects of Temperature, Pressure and Doping on Stoichiometry and Atomic Structure of Materials: Bulk, Surfaces and Clusters*
Oct 2014	CRC Symposium, FHI, Berlin, Germany *Adsorbate-Adsorbate Interactions on Surfaces at Realistic Conditions: A First-Principles Study*
May 2015	FHI-Workshop on Current Research Topics at the FHI, Potsdam, Germany *Activation of Small Molecules at Ni-Doped MgO Surfaces: An ab initio Study*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Periodic Systems*
Jul 2015	Summer School of the Max Planck-EPFL Center for Molecular Nanoscience and Technology, Schloss Ringberg, Kreuth, Germany *Defects in Solids*
Sep 2015	Psi-k 2015 Conference, San Sebastian, Spain *Defect-Defect Interaction at Surfaces and Interfaces at Realistic Conditions: Global Versus Local Effects of Doping*

Norina Richter

Jan 2014	Seminar, Theoretische Chemie, Technische Universität München, Munich, Germany *Importance of Space-Charge Effects for Concentration and Charge State of Defects at Metal-Oxide Surfaces*
Feb 2014	17th Meeting of the Fachbeirat of the Fritz-Haber-Institut, Berlin, Germany *Space-Charge Transfer at Intrinsic Defects and at (Organic) Adsorbates at Metal-Oxide Surfaces*
May 2014	Workshop on Catalysis from First Principles 2014, Institute of Theoretical Chemistry, Ulm University, Ulm, Germany *Charge-Carrier Doping Effects on Concentrations of Defects at Metal-Oxide Surfaces*

Patrick Rinke

Oct 2013	Colloquium of the Collaborative Research Centre “Hybrid Inorganic/Organic Systems for Opto-Electronics” (SFB 951- HIOS), Berlin, Germany *ZnO-Based Inorganic/Organic Systems from First Principles*
Nov 2013	Seminar, Aalto University, Helsinki, Finland *Hybrid Inorganic/Organic Interfaces from First Principles*
Jan 2014	International Workshop on Computational Physics and Materials Science, École polytechnique fédérale de Lausanne (EPFL), Lausanne, Switzerland

	Space-Charge Transfer in Hybrid Inorganic-Organic Systems
Jun 2014	Seminar, University of Luxembourg, Luxembourg *Space-Charge Transfer in Hybrid Inorganic-Organic Systems*
Jul 2014	ICMR Workshop on Ab-Initio Description of Charged Systems and Solid/Liquid Interfaces for Semiconductors and Electrochemistry, University of California, Santa Barbara, CA, USA *Space-Charge Transfer in Hybrid Inorganic-Organic Systems*
Jul 2014	IPAM Workshop, Density Functional Theory and Beyond: Computational Materials Science for Real Materials, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Excited-State Properties*
Aug 2014	International Conference, Condensed Matter in Paris 2014, Paris, France *Charge Transfer in Organic and Hybrid Organic/Inorganic Systems from First Principles*
Nov 2014	Autumn School on Basics of Electronic Structure Calculations, Tampere University of Technology, Tampere, Finland *Many-Body Theory and the GW Approximation*
Feb 2015	Symposium on Hybrid Inorganic/Organic Systems for Opto-Electronics (HIOS Symposium 2015), Berlin, Germany *Space-Charge Transfer in Hybrid Inorganic-Organic Systems*
Feb 2015	Workshop, Towards Reality in Nanoscale Materials VIII, Levi, Finland *Tackling the Charge-Transfer Problem with First Principles*
Mar 2015	APS March Meeting 2015, American Physical Society, San Antonio, TX, USA *Towards a Unified Description of Ground and Excited State Properties: GW vs RPA and Beyond*
May 2015	Physics Colloquium, University of Jyväskylä, Jyväskylä, Finland *Quantum Perspective of Novel Hybrid Materials*
Jul 2015	28th International Conference on Defects in Semiconductors, Helsinki, Finland *Space-Charge Transfer and Charged Defects at Surfaces*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Prediction of Electronic Spectra from First Principles*
Aug 2015	CECAM Summer school, Electronic structure at the cutting edge with the Elk code, Lausanne, Switzerland *Hedin Equations and GW Method*
Aug 2015	XXIV International Materials Research Congress 2015, Cancún, Mexico *Tackling the Charge Transfer Problem in Organic Systems and at Organic/Inorganic Interfaces from First Principles*
Sep 2015	Psi-k 2015 Conference, San Sebastian, Spain *To GW and Beyond: What We Can Learn from Molecular Calculations*

Angel Rubio

Oct 2013	Workshop on Modeling Single-Molecule Junctions: Novel Spectroscopies and Control, Berlin, Germany *Light-Induced Dynamical Processes in Finite and Extended Systems from TDDFT*
Nov 2013	Science Dissemination Talk, Nanotecnología, Fundación Valenciana de Estudios Avanzados, Valencia, Spain *Impacto de La Teoría En Nanociencia: Nuevos Materiales Y Dispositivos*
Nov 2013	The "March" Meeting, A Symposium in Honor of Norman H. March, Namur, Belgium *Non Linear Processes in Low Dimensional Systems within Time-Dependent Density Functional Theory*
Jan 2014	6th International Workshop and School on Time-Dependent Density-Functional Theory: Prospects and Applications, Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spain *Open Session about Challenges and Standing Problems*
Jan 2014	VI International Conference BIFI-2014: Exploring the Role of Computation in Science: From Biology to Physics, Zaragoza, Spain *Light-Induced Processes in Finite and Extended Systems from TDDFT*
Feb 2014	Colloquium of the Institute of Physical and Theoretical Chemistry, University of Würzburg, Würzburg, Germany *Non Equilibrium Dynamical Processes in Low Dimensional Systems from Time-Dependent Density Functional Theory*
Feb 2014	Colloquium of the Instituto de Ciencia de Materiales de Madrid (ICMM), Madrid, Spain *Multi-Scale Modeling in Chemistry and Materials Science: Combining Classical and Quantum Mechanics*
Mar 2014	APS March Meeting 2014, American Physical Society, Denver, CO, USA *Extensions of Density Functional Theory Approaches to Treating Quantum Phenomena and Quantum Entanglement*
Mar 2014	Colloquium, Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain *Modeling Energy Materials from First Principles Simulations: Optoelectronic and Hybrid-Photovoltaic Devices*
May 2014	Workshop on Materials Challenges in Devices for Fuel Solar Production and Employment, International Centre for Theoretical Physics, Trieste, Italy *Understanding Light-Induced Processes in Energy Materials from First Principles TDDFT Simulations*
Jun 2014	2nd Workshop on Surfaces, Interfaces and Functionalization Processes in Organic Compounds and Applications, (SINFO), Trieste, Italy *Non Equilibrium Light-Induced Dynamical Processes in Energy Materials*
Jun 2014	Colloquium Physikalische Chemie, Department Chemie, Ludwig-Maximilians-Universität München, Munich, Germany *Modeling Optoelectronic and Hybrid-Photovoltaic Devices within TDDFT*

Jun 2014	International Workshop, White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back St. Petersburg, Russia *Hybrid-Organic Photovoltaic Devices from First Principles Simulations*
Jun 2014	Seminar, Physical Chemistry Department (ISIC), École polytechnique fédérale de Lausanne (EPFL), Lausanne, Switzerland *Optoelectronic and Hybrid-Photovoltaic Devices from First Principles Simulations*
Aug 2014	Colloquium, Department of Physics, Stanford University, Stanford, CA, USA *Ab Initio Modelling of Light-Induced Non Equilibrium Dynamical Processes in Organic Materials*
Sep 2014	Applied Mathematics Seminar, Department of Mathematics, University of California, Berkeley, CA, USA *Efficient Implementation of Time-Dependent Density-Functional Theory to Treat Non-Linear Dynamical Processes in Molecular Nanostructures and Solid*
Sep 2014	Colloquium Molecular Foundry, Lawrence Berkeley Laboratory, Berkeley, CA, USA *Non Equilibrium Dynamical Processes in Organic Photovoltaic Applications*
Sep 2014	Colloquium, Department of Chemistry, University of California, Berkeley, CA, USA *First Principles Modeling of Photovoltaic and Optoelectronic Devices: Fundamentals and Applications*
Sep 2014	Physical Seminar, University of Rochester, Rochester, NY, USA *Modeling Non Equilibrium Dynamical Processes in TDDFT: Optoelectronic and Photovoltaic Applications*
Oct 2014	7th European School on Molecular Nanoscience (ESMolNa 2014), Gandia, Spain *Theoretical Spectroscopy: TDDFT*
Dec 2014	2014 Fall MRS Meeting and Exhibit, Materials Research Society, Boston, MA, USA *Novel Electronic and Structural Properties of Two-Dimensional Materials: Silicene, Germenene and Stanene*
Feb 2015	5th Symposium/Workshop of Computational Sciences (SWOCS-5), Pohang, South Korea *Simulation of Photon-Matter Interactions within QED-TDDFT*
Feb 2015	Colloquia, Center for Multidimensional Carbon Materials, Institute of Basic Sciences (IBS), UNIST Campus, Ulsan, South Korea *Non Equilibrium Dynamical Processes in TDDFT: Optoelectronic and Photovoltaic Applications*
Feb 2015	Colloquia, Center for Multidimensional Carbon Materials, Institute of Basic Sciences (IBS), UNIST Campus, Ulsan, South Korea *Novel Electronic and Structural Properties of Two Dimensional Materials: From Carbon-Nanostructures to Silicene*

Jul 2015	Theory Group Meeting, European XFEL, Hamburg, Germany *Ab-initio Simulations of Light-Matter Interactions*
Aug 2015	International Conference on High Pressure Science and Technology, Joint AIRAPT-25 & EHPRG-53, Madrid, Spain *Pressure Induced Phase Transition in Correlated Oxides and Simple Metals: Mott and Charge-Transfer Insulators*
Sep 2015	3rd International Conference on Correlation Effects in Radiation Fields CERF2015, Rostock, Germany *Quantum Electrodynamical Time-Dependent Density Functional Theory (QEDFT): An Ab-initio Framework for the Simulation of Photon-Matter Interactions*
Sep 2015	Chemistry, Materials & Light (CM&L 2015), International Year of Light, Bologna, Italy *Simulating Light-Induced Dynamical Processes in Light Harvesting Complexes*

Matthias Rupp

May 2015	CECAM/Psi-k Workshop, From Many-Body Hamiltonians to Machine Learning and Back, Berlin, Germany *Representing Atoms in Molecules*
Jun 2015	IPAM Workshop on Materials for a Sustainable Energy Future, Reunion Meeting, Institute for Pure and Applied Mathematics, Lake Arrowhead, CA, USA *Machine Learning for Materials Science*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Quantum Mechanics / Machine Learning Models*
Jul 2015	Seminar, Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany *Machine Learning for Quantum Chemistry*

Matthias Scheffler

Nov 2013	IPAM Program, Materials for a Sustainable Energy Future, Workshop IV: Energy Conservation and Waste Heat Recovery, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Lecture, Fuels from Sunlight - Potential and Challenges*
Jan 2014	Conference, Electronic Materials and Applications, The American Ceramic Society, Orlando, FL, USA *Big Data of Materials Science from First Principles - Critical Next Steps*
Jan 2014	Symposium on Surface and Nano Science 2014 (SSNS'14), Furano, Japan *Space-Charge Transfer at Defects and (Organic) Adsorbates at Metal-Oxide Surfaces*
Feb 2014	International Workshop on Advanced Materials 2014, Ras al Khaimah, UAE *Big Data of Materials Science from First Principles - Critical Next Steps*

Mar 2014	APS March Meeting 2014, American Physical Society, Denver, CO, USA *Hybrid Density Functionals Tuned Towards Fulfillment of Fundamental DFT Conditions*
Apr 2014	Shanghai Conference on Theoretical & Computational Chemistry, Shanghai, China *Big Data of Materials Science from First Principles - Critical Next Steps*
May 2014	FHI-Workshop on Current Research Topics at the FHI, Potsdam, Germany *Big Data of Materials Science from First Principles - Critical Next Steps*
May 2014	Wiener Physikalisches Kolloquium, Fakultät für Physik, University of Vienna, Vienna, Austria *Big Data of Materials Science from First Principles - Critical Next Steps*
Jun 2014	Interface Chemistry of Materials, PIRE-ECCI, Summer School, Shanghai, China *Big Data of Materials Science from First Principles - Critical Next Steps*
Jun 2014	Seminar, University of Science and Technology of China, Hefei, China *Big Data of Materials Science from First Principles - Critical Next Steps*
Jul 2014	Exciting Workshop Big Data of Materials Science from First Principles, Berlin, Germany *Electronic Structure Theory: Status and Outlook*
Jul 2014	IPAM Workshop, Density Functional Theory and Beyond: Computational Materials Science for Real Materials, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Electronic Structure Theory: Status and Outlook*
Jul 2014	IPAM Workshop, Density Functional Theory and Beyond: Computational Materials Science for Real Materials, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *IPAM Overview: Electronic Structure Theory for the Ground State*
Jul 2014	KOSMOS Summer University, Humboldt-Universität zu Berlin, Berlin, Germany *Electronic Structure Theory: Status and Outlook*
Aug 2014	248th ACS National Meeting and Exposition, American Chemical Society, San Francisco, CA, USA *Space-Charge Transfer at Intrinsic Defects and at (Organic) Adsorbates at Metal-Oxide Surfaces*
Aug 2014	FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany *Big Data of Materials Science from First Principles - Critical Next Steps*
Sep 2014	Seminar, University of Connecticut, Storrs, CT, USA *Big Data of Materials Science from First Principles - Critical Next Steps*
Oct 2014	The 4th International Workshop on Quantum Energy, Chengdu, China *Big Data of Materials Science from First Principles - Critical Next Steps*
Nov 2014	The 17th Asian Workshop on First-Principles Electronic Structure Calculations, Seoul, South Korea *Big Data of Materials Science from First Principles - Critical Next Steps*

Dec 2014	2014 Fall MRS Meeting and Exhibit, Materials Research Society, Boston, MA, USA *Big Data of Materials Science from First Principles - Critical Next Steps*
Jan 2015	CPTS Data Driven Sciences Round Table, Tübingen, Germany *Big Data Analytics in CPT Science*
Feb 2015	IPAM Workshop, Machine Learning for Many-Particle Systems, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Big Data of Materials Science - Critical Role of the Descriptor*
Apr 2015	Symposium on the Occasion of the Retirement of Prof. Dr. Oleg Pankratov, Quantum Theory of Materials, Erlangen, Germany *Big Data of Materials Science - Critical Next Steps*
May 2015	Kolloquium, SFB 840 "Von Partikulären Nanosystemen zur Mesotechnologie", Bayreuth, Germany *Big Data of Materials Science -- Critical Role Next Steps*
May 2015	Workshop, Computer Simulations for Condensed Phase Systems: From Correlated Electrons to Novel Materials, Rome, Italy *Big Data of Materials Science - Critical Role of the Descriptor*
Jun 2015	IPAM Workshop on Materials for a Sustainable Energy Future, Institute for Pure and Applied Mathematics, Lake Arrowhead, CA, USA *Metal Oxides with Defects and Interfaces: Materials for Energy Conservation, Conversion, and Storage*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Electronic Structure Overview*
Jul 2015	Summer School of the Max Planck-EPFL Center for Molecular Nanoscience and Technology, Schloss Ringberg, Kreuth, Germany *Big Data Analytics, Novel Materials Discovery*
Sep 2015	6th International Conference on Nanoscience and Technology (ChinaNANO 2015), Beijing, China *Big-Data Analytics for Materials Science: Concepts, Challenges and Hype*
Sep 2015	CeNS Workshop 2015 "Channels and Bridges to the Nanoworld", Venice, Italy *Big Data and Data Analytics for Materials Science*

Honghui Shang

Apr 2014	Team Meeting on ETSF Electron-Phonon Coupling, Zeuthen, Germany *Density-Functional Perturbation Theory for Lattice Dynamics with Numeric Atom-Centered Orbitals*
Jun 2014	International Workshop, White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back, St. Petersburg, Russia *Density-Functional Perturbation Theory for Lattice Dynamics with Numeric Atom-Centered Orbitals*
Aug 2014	FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany *Density-Functional Perturbation Theory for Lattice Dynamics in FHI-aims*

Jan 2015 Team Meeting on ETSF Electron-Phonon Coupling, Rome, Italy
First-Principles Evidence for Intermediate Hole Polaron in ZnO

Alexandre Tkatchenko

Nov 2013 International Symposium on Computational Sciences (ISCS2013), Shanghai, China
Collective van der Waals Interactions in Molecules and Solids

Nov 2013 Retreat, Intelligent Data Analysis Group, Technische Universität Berlin, Berlin, Germany
First-Principles Atomistic Modeling: Pushing the Limits of Accuracy and Efficiency

Nov 2013 Seminar, Jilin University, Changchun, Jilin, China
First-Principles Atomistic Modeling: Pushing the Limits of Accuracy and Efficiency

Dec 2013 CECAM Workshop, Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality, Tel Aviv University, Tel Aviv, Israel
Collective Phenomena in Organic Materials Described with Coupled Quantum Harmonic Oscillators

Jan 2014 CECAM Workshop, Two-dimensional inorganic materials (2DIM): property simulations from band structure to devices, Lausanne, Switzerland
van der Waals Interactions in Nanostructures: Breaking Preconceived Notions

Jan 2014 Colloquium, University of Bonn, Bonn, Germany
van der Waals Interactions in Nanostructures: Breaking Preconceived Notions

Mar 2014 Hauptvortrag, DPG-Frühjahrstagung, Dresden, Germany
The Many-Body Path Towards Quantitative Modeling of Complex Adsorption Systems

May 2014 Colloquium, Max Planck Institute for Polymer Research, Mainz, Germany
The Many-Body Path Towards Predictive Modeling of Complex Materials

May 2014 Colloquium, University of Luxembourg, Luxembourg
The Many-Body Path Towards Predictive Modeling of Complex Materials

May 2014 E-MRS Spring Meeting, Lille, France
van der Waals Interactions in Molecular Materials: Breaking Preconceived Notions

May 2014 FHI-Workshop on Current Research Topics at the FHI, Potsdam, Germany
Collective van der Waals Interactions in Materials

Jun 2014 Colloquium, University of Groningen, Groningen, The Netherlands
The Many-Body Path Towards Predictive Modeling of Complex Materials

Jun 2014 Physics Boat Workshop 2014, Helsinki, Finland/Stockholm, Sweden
van der Waals Interactions in Molecular Materials: Breaking Preconceived Notions

Jun 2014	Workshop, Many-Body Interactions: From Quantum Mechanics to Force Fields, Telluride Science Research Center, Telluride, CO, USA *Many-Body van der Waals Dispersion: Strong Correlations in Weak Interactions?*
Jul 2014	IPAM Workshop, Density Functional Theory and Beyond: Computational Materials Science for Real Materials, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *van der Waals Interactions in DFT*
Aug 2014	CAMD Summer School on Electronic Structure Theory and Materials Design, DTU Department of Physics, Lyngby, Denmark *Many-Body van der Waals Dispersion: Strong Correlations in Weak Interactions?*
Aug 2014	FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany *From Dispersion Interactions to Farsighted Electron Correlation - A Unified Approach Based on Atomic Response Functions*
Sep 2014	16th European Seminar on Computational Methods in Quantum Chemistry (ESCMQC), Houffalize, Belgium *From Dispersion Interactions to Farsighted Electron Correlations – A Unified Approach Based on Atomic Response Functions*
Sep 2014	SMARTER4 Conference, Durham, UK *Structure, Stability, and Vibrations of Molecular Materials: The Role of (Many-Body) Dispersion Interactions*
Oct 2014	Colloquium, Department of Chemistry, UNIST Campus, Ulsan, South Korea *The Many-Body Path Towards Quantitative Modeling of Complex Molecules and Materials*
Oct 2014	Physical Seminar, Department of Chemistry, University of Rochester, Rochester, NY, USA *The Many-Body Path Towards Quantitative Modeling of Complex Molecules and Materials*
Oct 2014	Woodward Lecture, Harvard University, Cambridge, MA, USA *The Many-Body Path Towards Quantitative Modeling of Complex Molecules and Materials*
Oct 2014	Workshop of the SFB 658-Integrated Research Training Group, Lübbenau, Germany *The Many-Body Path Towards Quantitative Modeling of Complex Adsorption Systems*
Nov 2014	Colloquium, University of Bristol, Bristol, UK *The Many-Body Path Towards Quantitative Modeling of Complex Molecules and Materials*
Nov 2014	Seminar, Forschungszentrum Jülich, Jülich, Germany *Non-Additive Effects in Molecular Adsorption*
Dec 2014	Colloquium of the Collaborative Research Centre “Hybrid Inorganic/Organic Systems for Opto-Electronics” (SFB 951- HIOS), Berlin, Germany

	The Many-Body Path Towards Quantitative Modeling of Complex Adsorption Systems
Jan 2015	Colloquium, University of Rostock, Rostock, Germany *The Many-Body Path Towards Quantitative Modeling of Complex Molecules and Materials*
Jan 2015	Winter Workshop, Frontiers of Multiscale Modelling - Current Obstacles and New Horizons for Energy, Materials, and Catalysis, Stubachtal, Austria *van der Waals Correlations in Materials: Current Obstacles and New Horizons*
Feb 2015	IPAM Workshop, Machine Learning for Many-Particle Systems, Institute for Pure and Applied Mathematics, Los Angeles, CA, USA *Many Particles, Collective Variables and Machine Learning*
Apr 2015	Colloquium, Universitat de Barcelona, Barcelona, Spain *Non-Covalent van der Waals Interactions in Molecules and Materials*
Apr 2015	Seminar, Institute of Basic Science, Seoul, South Korea *The Many-Body Path Towards Quantitative Modeling of Complex Molecules and Materials*
Jul 2015	Colloquium, University of Luxembourg, Luxembourg *The Many-Body Path Towards Quantitative Modeling of Complex Molecules and Materials*
Jul 2015	Congress of Theoretical Chemists of Latin Expression, Torino, Italy *Quantum Fluctuation in Molecules*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Practical Approaches to van der Waals Interactions*
Aug 2015	Colloquium, The Rowland Institute at Harvard, Cambridge, MA, USA *van der Waals Interactions for Molecules on Surfaces: Weak or Strong?*
Aug 2015	Dynamics at Surfaces, Gordon Research Conference (GRC), Newport, RI, USA *van der Waals Interactions for Molecules at Surfaces*
Aug 2015	XXIV International Materials Research Congress 2015, Cancún, Mexico *Quantum Fluctuations in Molecules and Materials*
Sep 2015	EUROMAT 2015, European Congress and Exhibition on Advanced Materials and Processes, Warsaw, Poland *Quantum Fluctuations in Molecular Materials*
Sep 2015	Psi-k 2015 Conference, San Sebastian, Spain *Non-Covalent Interactions in Density-Functional Theory*

Igor Ying Zhang

Jun 2014	International Workshop, White Nights of Materials Science: From Physics and Chemistry to Data Analysis, and Back, St. Petersburg, Russia *Toward Simple Orbital-Dependent Density Functionals for Molecular Dissociation*
Aug 2014	FHI-aims Developers' and Users' Meeting, Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals, Berlin, Germany *Assessment of Density Functionals in FHI-aims: Searching for the Next-Generation Density Functional with a Broader Application*
Jun 2015	Workshop, Methods and Algorithms in Electronic-Structure Theory, Schloß Ringberg, Kreuth, Germany *Explore Efficient Orbital-Dependent Density Functionals for a Broader Application*
Jul 2015	Hands-on Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials, Berlin, Germany *Test Sets and Benchmark Techniques for Materials Science*
Sep 2015	Psi-k 2015 Conference, San Sebastian, Spain *Test Set for Materials Science and Engineering*

ERC Group on Organic Functional Materials and Intermolecular Interactions **Head: Alexandre Tkatchenko**

Guest scientists, staying for at least six months:

Wei Liu	*until 01/02/2015*	*ERC*
Wang Gao	*until 31/07/2014*	*ERC*
Mausumi Chattopadhyaya		*AvH*
Fairoja Cheenicode Kabeer		*Harvard EFRC*
Gionni Marchetti		*DFG*
Igor Poltavsky		*ERC*
Limin Zheng		*China Scholarhsip Council (CSC)*

Graduate students: 6 (2 from external funds, CSC and Harvard EFRC)

General Remarks

The ERC (European Research Council) Research Group *Organic Functional Materials and Intermolecular Interactions*, lead by Alexandre Tkatchenko, was established in May 2010 and is hosted by the Theory Department. This group performs fundamental developments of efficient first-principles methods for an accurate modeling of non-covalent interactions in molecules, solids, and interfaces. The developed methods are applied to a wide range of fundamental complex materials, aiming at understanding their qualitative and quantitative structural, cohesive, and electronic properties at the atomic scale. The group currently consists of 5 postdoctoral researchers, and 5 PhD students, together with the PI.

Since the group was established, several postdoctoral researchers and one PhD students have left for academic and industry positions elsewhere. Dr. Wei Liu accepted an offer for full professor in the University of Science and Technology in Nanjing, China (2014). Dr. Wang Gao took an associate professor position in Jilin University, China (2014). Dr. Guo-Xu Zhang took a position as lecturer at Harbin Institute of Technology in China (2015). Dr. Anthony Reilly became a Senior Design Centre Scientist at Cambridge Crystallographic Database Centre (CCDC), UK (2014). Dr. Katja Hansen took a Scientist position at 3M, Duesseldorf (2014). Currently, 3 PhD students (Vivekanand V. Gobre, Victor G. Ruiz, and Nicola Ferri) are in process of submitting their theses. These successful career developments of former and current ERC group members highlight the high quality of the research and scientific training in the group.

Scientific Scope

Non-covalent van der Waals (vdW) interactions are ubiquitous in nature, making the existence of molecular liquids and solids possible; controlling protein-protein and drug-protein binding inside our cells; and giving geckos the ability to "defy gravity" and climb on walls and ceilings. An accurate description of vdW interactions is extremely challenging, since the vdW dispersion energy arises from collective motion of electrons and must be described by many-electron quantum mechanical methods. The lack of accurate and efficient methods for capturing vdW interactions in large and complex systems hinders truly quantitative predictions of properties and functions of technologically relevant materials. The ERC group has successfully addressed this challenging age-old problem, by developing a hierarchy of efficient and advanced quantum-mechanical methods with accuracy and capacity to predict new phenomena in complex materials of fundamental and technological interest. These developments are based on a combination of techniques developed in different fields, such as many-body physics, statistical mechanics, chemistry, and computer science. The methods developed by the group are now widely used worldwide to enable molecular simulations with predictive power for large and complex materials, chemicals, and biological systems.

Research Highlights

Wavelike Nature of van der Waals Interactions at the Nanoscale

With the increasing focus on supramolecular chemistry and nanostructured materials, vdW interactions are being employed and probed at increasingly larger scales and decreasing dimensionality. However, our current understanding of these interactions is largely based on small model systems and idealized pairwise London dispersion picture. As a result of this inconsistency, predictions of both static and dynamic properties of nanoscale structures may fail in quantitative and sometimes even qualitative manner.

We demonstrated that in supramolecular complexes and low-dimensional nanostructures, vdW correlations are more naturally described in terms of coupling between fluctuating dipole waves. This leads to several nontrivial effects in vdW interactions that cannot be explained by dispersion corrections and non-local functionals based on electron density, but that are correctly captured by our developed many-body dispersion (MBD) model. In linear chain structures and layered 2D materials, the interaction energy shows complex power laws that can be systematically tuned from insulating to metallic behavior. The associated wave fluctuations are largely

delocalized over the whole system, continuously changing the interaction power law as a function of the separation between nanostructures. For molecules interacting through nanostructures, we observe a regime in which their interaction energy *increases*, instead of decreasing as naively expected from dielectric screening. Further application to carbon-based supramolecular complexes demonstrates that omitting wavelike vdW fluctuations leads to differences in association constants of up to five orders of magnitude where there should be degeneracy according to high-level quantum Monte Carlo calculations.

Taken together, our findings indicate that the wavelike nature of vdW interactions provides a hitherto unexplored avenue that could be used for tailoring the assembly of complex polarizable systems at the nanoscale.

Modeling Quantum Nuclei with Perturbed Path Integral Molecular Dynamics

The quantum nature of nuclear motions plays a vital role in the structure, stability, and thermodynamics of molecules and materials. Whenever interatomic forces are strong, nuclear quantum fluctuations (NQF) can be fairly pronounced at room temperature and even above it. The standard approach to model NQF in chemical and biological systems is path-integral molecular dynamics (PIMD). Unfortunately, conventional PIMD simulations can have exceedingly large computational cost due to the need of employing an excessive number of coupled classical subsystems (beads) for quantitative accuracy. Hence, the development of a non-empirical method for NQF, which is both accurate and efficient, would be desirable.

To achieve this challenging goal we combined perturbation theory with Feynman-Kac imaginary-time path integral approach to quantum mechanics and derive improved non-empirical partition function and estimators to calculate converged quantum observables. Our *perturbed path-integral* (PPI) method requires the same ingredients as conventional approaches, but increases the accuracy and efficiency of path integral simulations by an order of magnitude. Any kind of phase sampling technique, and any thermostat or barostat can be utilized. The converged observables can be obtained either *on-the-fly* or *a posteriori* conventional PIMD simulations, which are utilized as a base of the developed PPI approach.

Applications were carried out for thermodynamics of a quantum harmonic oscillator and double-wall potential, empirical water model containing 256 water molecules within periodic boundary conditions, *ab initio* simulations of nitrogen and benzene molecules, and graphene. For all of these examples, our PPI approach with 4 to 8 classical beads recovers the nuclear

quantum contribution to the total energy and heat capacity at room temperature within 3% accuracy, paving the way toward seamless modelling of nuclear quantum fluctuations in realistic molecules and materials.

Electronic Properties of Molecules, Surfaces, and Interfaces with a Self-Consistent Interatomic van der Waals Density Functional

How strong is the effect of long-range vdW interactions on the electronic properties of molecules and extended systems? It is often argued that the vdW energy has a small, or even negligible, influence on the electron density and derived electronic properties, since the vdW energy represents only a tiny fraction (0.001%) of the total electronic energy.

To answer the question posed above, we derived a fully self-consistent (SC) implementation of the density-dependent interatomic vdW functional of Tkatchenko and Scheffler and its extension to surfaces. Not surprisingly, vdW self-consistency leads to tiny modifications of the structure, stability, and electronic properties of molecular dimers and crystals. However, unexpectedly large effects were found in the binding energies, distances and electrostatic moments of highly polarizable alkali metal dimers. Most importantly, vdW interactions produced complex and sizable electronic charge redistribution in the vicinity of metallic surfaces and at organic/metal interfaces. As a result, for several coinage metal (111) surfaces, self-consistency induces modifications in the surface dipole, leading to an increase of up to 0.30 eV in the computed workfunctions. Furthermore, in the case of HIOS, SC vdW entails modifications of up to 0.22 eV in the shift of the interface workfunction, a property induced by molecular adsorption. The underlying mechanism responsible for the workfunction modifications stems from an interplay between two effects driven by SC vdW interactions: (i) the modification of the interface dipole, and (ii) a reduction in the charge transfer between the molecule and the surface.

The analysis of SC vdW effects demonstrated the important effect of vdW interactions on the electronic properties of different classes of systems, with self-consistency systematically improving the agreement between the theoretical predictions and the experimental measurements. Our work revealed a nontrivial connection between electrostatics and long-range electron correlation effects.

Essential Role of van der Waals Interactions in the Structure, Stability, and Catalytic Processes for Molecules at Surfaces

Hybrid inorganic/organic systems (HIOS) often possess collective electronic, optical, vibrational, and catalytic properties that the separate components forming the interface do not exhibit. These novel interface properties stem from a subtle interplay between a range of covalent and non-covalent interactions. In particular, van der Waals (vdW) dispersion interactions play an essential role in many properties of HIOS, including their structure and stability, and sometimes even their electronic properties and reactivity.

We made systematic efforts in developing efficient first-principles methods that enable quantitative modeling and new qualitative insights into the structure and stability of HIOS. Our DFT+vdW^{surf} method synergistically combines Lifshitz-Zaremba-Kohn theory with intermolecular perturbation techniques, demonstrating that the collective response of the substrate electrons can modify vdW coefficients in HIOS by up to an order of magnitude. Calculations using this method have shown that the inclusion of collective vdW effects is essential to cover a wide range of interactions in the adsorption of molecules on surfaces. The critical role of screened vdW interactions in the structure and stability of HIOS has implications in catalysis, as demonstrated by the relative stability of reactive intermediates in oxygen-assisted reactions in catalytic systems such as amides, isopropoxys, thiolates, and acetylides on the Au(111) surface.

Further gain in accuracy and conceptual understanding of HIOS is possible by applying the recently developed many-body dispersion (MBD) method. This method allows us to capture anisotropic polarization effects in HIOS and demonstrate strong non-additivity in vdW interactions for atoms, molecular assemblies, and nanostructures adsorbed on metal surfaces. The application of the MBD method enables us to go beyond single molecules on surfaces and efficiently address many-body interactions in dense adsorbed molecular layers, which is necessary to understand the assembly of complex nanostructures on surfaces.

Third-Party Funded Projects

- ERC – European Research Council, Starting Grant: Van der Waals Interactions in Complex Materials; A. Tkatchenko – since 2011.

- DFG – German Research Foundation, SPP 1807 Control of London dispersion interactions in molecular chemistry, spokesperson: Peter R. Schreiner; A. Tkatchenko – since 2015.

- DFG – German Research Foundation, Basis module, project: Exploring Chemical Com-

pound Space with Machine Learning; A. Tkatchenko, K.-R. Müller – since 2014.

- DOE – US Department of Energy, EFRC (Energy Frontier Research Centers): Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC), coordinator: C. Friend; A. Tkatchenko – since August 2014.

- DFG – German Research Foundation, SFB 951, Hybrid Inorganic/Organic Systems (HIOS), spokesperson: Norbert Koch; A. Tkatchenko, M. Scheffler – since 2015.

- INCITE computer time allocation for 300 million CPU hours // Argonne National Laboratory and Oak Ridge National Laboratory (with D. Alfe, A. Michaelides, K. Jordan, M. Gillan), 2013-2015.

Organization of workshops and conferences

- Organizer of the focused session "Van der Waals Interactions in Complex Materials: Bridging Theory and Experiment" at the APS March Meeting 2014, Denver, USA (with R. A. DiStasio Jr.).

- Organizer of a CECAM workshop "Addressing Challenges in First-Principles Based Modeling of Molecular Materials" (with A. Reilly and M. Ceriotti).

- Organizer of IPAM workshop "Machine Learning for Many-Particle Systems", Institute for Pure and Applied Mathematics, UCLA, USA, 2015 (with A. Aspuru, G. Csanyi, and K. R. Mueller).

- Organizer of CECAM workshop "From Many-Body Hamiltonians to Machine Learning and Back", Berlin, Germany, May 2015 (with M. Rupp).

- Organizer of the workshop "Modeling Many-Body Interactions (MMBI 2015)", Lake Garda, Italy, May 2015 (with R. A. DiStasio Jr., A. Ambrosetti, and P. Silvestrelli).

- Proponent and main organizer of a semester program "Understanding Many-Particle Systems with Machine Learning", Institute for Pure and Applied Mathematics, UCLA, USA (approved for Fall 2016). Co-organizers: Klaus-Robert Mueller (TU-Berlin), Gabor Csanyi (Cambridge), Alan Aspuru-Guzik (Harvard), Marina Meila (U. Washington).