Curriculum Vitae
and
List of Publications

Prof. Dr. rer. nat. Peter Blöchl

June 18, 2022

Business Address

Institute for Theoretical Physics
Clausthal University of Technology
Leibnizstr. 10
D-38678 Clausthal-Zellerfeld
Germany
Phone: +49-(5323)-722021
Fax: +49-(5323)-723116
Email: peter.bloechl@tu-clausthal.de
WWW: http://www.pt.tu-clausthal.de/atp/

Research Interests

My research aims at the prediction of materials properties from fundamental physical principles. The elementary building blocks considered are nuclei and electrons, held together by electrostatics. To make the equations tractable I resort to density functional theory (Nobel prize Walter Kohn, 1998), ab-initio molecular dynamics (Car and Parrinello, 1985) and the projector augmented wave method (Blöchl, 1994). With my computer code CP-PAW, I study solid-state reactions relevant for microelectronic applications, energy conversion, the function of catalysts and enzymatic reaction mechanisms in biochemistry.

Overview

5 awards
$>$ 100 publications (8 patents, 1 Nature)
$>$ 60,000 citations
h-index of 44[1] (44 publications that are cited at least 44 times)
One paper is among the top 100 of the most cited scientific publications[2] and it is the ninth-most-cited paper out of more than 500,000 published in the 120-year history of *Physical Review*. [3]

---

[1] ResearcherID B-3448-2012, Dec. 21
[2] R. van Noorden, B. Maher and R. Nuzzo, Nature 514, 550 (2014)
[3] Oct. 15, 2014, search in the *Physical Review Online Archive* with criteria "a-z".

Honors and Awards

since 04/2003	Member of the Braunschweigische Wissenschaftliche Gesellschaft (Academy of Sciences)
06/2000	IBM Invention Achievement Award: Second Plateau.
11/1998	IBM Invention Achievement Award: First Plateau.
04/1998	IBM First Patent Application Invention Achievement Award for the patent entitled "Material with Reduced Optical Absorption".
1995	Visiting Professor at the Vienna University of Technology, summer-term 1995.
11/1993	IBM Outstanding Technical Achievement Award for the development and validation of novel classical and quantum simulation methods to complex molecular systems.
08/1990	"Young Author Best Paper Award", 20th International Conference on the Physics of Semiconductors, Thessaloniki, Greece.

Education and Degrees

04/1997	Habilitation, Vienna University of Technology, Austria. Venia legendi for "Theoretical Physics". Thesis entitled "The Projector Augmented Wave Method"
03/1989	Doctorate degree in natural science (Dr. rer. nat.), University of Stuttgart, Germany. Thesis entitled "Total Energies, Forces and Metal-Semiconductor Interfaces". Advisor: Prof. O.K. Andersen (Max Planck Institute, Stuttgart).
10/1985-09/1988	Graduate studies, University of Stuttgart, Germany.
07/1984	"Diploma" degree in physics, University of Karlsruhe, Germany; Thesis entitled "Criterion for Global Stability in Open Systems"; Advisor: Prof. A. Schmid.
10/1978- 09/1984	Study of physics, University of Karlsruhe, Germany.
04/1978	Abitur (Final high school degree)
08/1969-04/1978	High school, Karlsruhe, Germany
1966-1968	Elementary school, Karlsruhe, Germany

Professional Appointments

since 10/2000	Full Professor (C4) at the Clausthal University of Technology, Germany.
10/1990-09/2000	Research staff member, IBM Zurich Research Laboratory, Ruschlikon, Switzerland.
03/1989-09/1990	Research associate, IBM Thomas J. Watson Research Center, Yorktown Heights, NY, (With Prof. S.T. Pantelides). (Leave of absence from the Max Planck Institute for Solid State Research from 03/1989-08/1990)
01/1988-08/1990	Research staff member, Max Planck Institute for Solid State Research, Stuttgart, Germany, (With Prof. O.K. Andersen).
12/1984-12/1987	Research staff member, Max Planck Institute for Metals Research, Stuttgart, Germany. (With Prof. H. Fischmeister)
1983-1984	Teaching assistant, University of Karlsruhe, Germany.

Other professional activities

since 10/2013	Member of the managing committee of the Collaborative Research Center SFB1073 "Atomic scale control of energy conversion"
07/2010	Member of the scientific committee for the symposium "Post-Si CMOS Electronic Devices: The Role of Ge and III-V Materials" at the E-MRS Meeting June 7-11, 2010 in Strasbourg, France.
03-12/2007	Participation in a course for the development of management skills (13 days).
09/2007	Symposium co-chair at the "10th International Conference on Advanced Materials (ICAM2007)" of the "International Union of Materials Societies", Symposium "Computational Materials Science", Oct 8-13, 2007, Bangalore,India.
06/2006	Co-organizer for the CECAM Workshop "State of the art, developments and perspectives of electronic structure calculations in the frame of the Projector Augmented-Wave (PAW) method." with F. Jollet, N. Holtzwarth and J.J. Mortensen.
07/2005	Referee for the DFG priority program "First-Principles Methods"
04/2005-03/2011	Member of the Fakultätsrat Physik, Chemie und Materialwissenschaften of Clausthal University of Technology

09/2004	Referee for DFG research group "SiC als Halbleitermaterial: Alternative Wege in Züchtung und Dotierung", Erlangen, Germany
08/2004-03/2009	Member of the Board of the "Simulationswissenschaftliche Zentrum" at Clausthal University of Technology.
2004-2007	Member of the Technical Program Committee of the IEEE Semiconductor Interface Specialist Conference (SISC)
03/2003	Co-organizer of the ESF Exploratory Workshop "Growth, structure and electrical properties of high-k gate dielectrics: atomistic modeling vs. experiment", March 18-19, 2003; Ruschlikon, Switzerland.
01/2003	External examiner for the PhD Defense of Dr. Bernd Ensing, Free University of Amsterdam, The Netherlands.
07/2002-08/2002	Member of the Institute for Theoretical Physics, University of California, Santa Barbara, USA
04/2001	Referee for DFG research centers "Nanotechnology", Bonn, Germany
since 04/2001	Director "Institute of Theoretical Physics", Clausthal University of Technology, Germany
04/2001-03/2005	Member of the Fachbereichsrat Physik, Metallurgie and Werkstoffwissenschaften of Clausthal University of Technology
04/2001-03/2003	Member of the Mathematisch-Naturwissenschaftliche Fakultätrat of Clausthal University of Technology Werkstoffwissenschaften of Clausthal University of Technology
since 03/2001	Member of the Advisory board of SWISSRISK, Zurich, Switzerland. (SWISSRISK offers financial risk evaluation on the internet)
12/2000	Examiner PhD of Brice Arnaud, University Louis Pasteur, Strasbourg, France.
12/2000	Co-examiner PhD of Hans-Martin Senn, ETH-Zurich, Switzerland.
since 04/1997	Lecturer (Univ.-Doz.), Institute for Physical Chemistry, Vienna University of Technology, Austria.
1997-1998	Consultant for DSM, The Netherlands.
09/1995	Vice-chairman, "European Research Conference on Electronic Structure of Solids: Itinerant Magnetism," Lunteren, The Netherlands.
05/1995-06/1995	Visiting Professor, Vienna University of Technology, Austria. Course on "Computer Simulations of Chemical Reactions and Molecular Dynamics."

1994-1997	Project leader of the node at the IBM Zurich Research Laboratory for the "Human Capital and Mobility Network" of the European Communities entitled "Ab-Initio (From Electronic Structure) Calculation of complex Processes in Materials".
1993	Co-editor of "Computations for the Nano-Scale", NATO ASI Series E: Applied Sciences; Vol. 240; ed. P.E. Blöchl, C. Joachim, A.J. Fisher (Kluwer, Dordrecht, 1993).
10/1992	Director, NATO Advanced Research Workshop "Computations for the Nano-Scale", Aspet, France.

Memberships

Braunschweigische Wissenschaftliche Gesellschaft (Academy of Sciences)
German Physical Society
Deutscher Hochschulverband

Refereeing

- Nature, Nature Materials, Science, Physical Review Letters, Physical Review B, Angewandte Chemie, Chemistry, IEEE Electron Device Letters, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of Physics, Organometallics, New Journal of Physics, Journal of Applied Physics,
- National Science Foundation (USA), Deutsche Forschungsgemeinschaft (Germany), Fonds zur Förderung der wissenschaftlichen Forschung (Austria)

Research contracts

7/2021-6/2025	"Relaxation, thermalization, and condensation in highly excited solids", Project B03 in the DFG Collaborative Research Centre SFB1073: "Atomic scale control of energy conversion". (3rd period)
7/2021-6/2025	"From electron transfer to chemical energy storage: first principles studies ofcorrelated processes", Project C03 in the DFG Collaborative Research Centre SFB1073: "Atomic scale control of energy conversion". (3rd period)
7/2017-6/2021	"Relaxation, thermalization, transport and condensation in highly excited solids", Project B03 in the DFG Collaborative Research Centre SFB1073: "Atomic scale control of energy conversion". (2nd period)
2015-2018	"Understanding the properties of the rare earth hexaborides - A synergistic approach based on spectroscopy and computational methods", DFG Research Grant.
7/2017-6/2021	"From electron transfer to chemical energy storage: first principles studies ofcorrelated processes", Project C03 in the DFG Collaborative Research Centre SFB1073: "Atomic scale control of energy conversion". (2nd period)
7/2013-6/2016	"Energies and forces for Materials with Strong Correlations", Project 9 of DFG Research Unit FOR1346: "Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials", (2nd period), 110,900 €.
10/2013-6/2017	"Relaxation, thermalization, transport and condensation in highly excited solids", Project B03 in the DFG Collaborative Research Centre SFB1073: "Atomic scale control of energy conversion" (1st period). 141,800 €
10/2013-6/2017	"From electron transfer to chemical energy storage: first principles studies ofcorrelated processes", Project C03 in the DFG Collaborative Research Centre SFB1073: "Atomic scale control of energy conversion" (1st period). 141,800 €
9/2012-8/2015	"Understanding size and Interface dependent anisotropic thermal conduction in correlated multilayer structures", Project in DFG Priority program SPP1386: "Nanostructured Thermoelectrics: Theory, model systems and controlled synthesis". 131,225 €.
7/2010-6/2013	"Energies and forces for Materials with Strong Correlations", Project 9 of DFG Research Unit FOR1346: "Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials", 132,000 €.

4/2009-3/2012	"Understanding size and Interface dependent anisotropic thermal conduction in correlated multilayer structures", Project in DFG Priority program SPP1386: "Nanostructured Thermoelectrics: Theory, model systems and controlled synthesis". (Consulting member)
9/2009-3/2012	"Energy Conversion Processes in Molecular Systems at Nano Contacts", Project 1 of the "NTH School for Contacts in Nanosystems". (3/4 position for 2.5 years.)
10/2007-09/2009	"Local Correlations in density functional theory using a mixed density and density matrix functional theory" Part of DFG Priority Program SPP1145: "Modern and Universal first-principles Methods for Many-Electron Systems in Chemistry and Physics", 88,200 €.
01/2006-12/2006	"Implementation of the COSMO model for solutions as periodic method in the PAW code" Research contract with a major Chemical Company, 60,000 €
04/2004-03/2005	"Ab-initio Simulationen zur Stickstofffixierung des Enzyms Nitrogenase", HLRN computertime for Project nic00003, 308,000 €
04/2004-03/2005	"Ab-initio Simulationen des Wachstums von High-K Oxiden auf Silizium", HLRN computertime for Project nip00002; 336,000 €
01/2004-12/2006	"Epitaxial technologies for Ultimate Scaling (ET4US)", EU Information Society Technologies Project 002048; 217,264 €, (Total EU contribution 3,727,000 €)
04/2003-03/2004	"Ab-initio Simulationen des Wachstums von High-K Oxiden auf Silizium", HLRN computertime for Project nip00002; 420,000 €
04/2003-03/2004	"Ab-initio Simulationen zur Stickstofffixierung des Enzyms Nitrogenase", HLRN computertime for Project nic00003; 140,000 €
07/2001-06/2004	"Integration of very high-k dielectrics with silicon CMOS technology (INVEST)", EU Information Society Technology Project (IST-2000-4.8.5); 227,520 €; (Total EU Contribution 1,903,566 €)
04/2001	Parallelrechner, Institute for Theoretical Physics, TU Clausthal, HBFG-144-148; 500,000 DM

Students, PhD students, Post-doctoral Fellows and Visiting Scientists

PhD students, Post-docs and Visiting scientists

2021-today	Lukas Rump (PhD Student, SFB1073, Georg August University, Göttingen)
2017-today	Michael Ten Brink, (PhD Student, SFB1073, Georg August University, Göttingen)
2016-2021	Florian Sohn, (PhD Student, DFG project, Georg August University, Göttingen)
-2016	Ebad Kamil, (PhD Student, FOR1346, Georg August University, Göttingen)
2013-1.2019	Robert Schade, (PhD Student, FOR1346, Georg August University, Göttingen)
6.2014-11.2018	Mohsen Sotoudeh, (PhD Student, SFB1073, Georg August University, Göttingen)
11.2013-6.2018	Sangeeta Rajpurohit, (PhD Student, SFB1073, Georg August University, Göttingen)
2011-7.2016	Ebad Kamil, (PhD Student, FOR1346, Georg August University, Göttingen)
12.2006-10.2012	Mattheus Uijttewaal (Post-doc, Clausthal University of Technology)
11.2006-11.2011	Christian Walther (PhD student, SPP1145 Clausthal University of Technology)
2004-2008	Andrei Reyes Huamantinco (PhD Student, EU project ET4US, Clausthal University of Technology)
2004-4.2008	Sascha Hemmen (PhD Student, Clausthal University of Technology)
2004-2008	Alexander Poddey (Diploma and PhD Student, Clausthal University of Technology)
2002-2004	Dr. Christopher Ashman (Post-doc, EU project INFOS)
2001-2004	Clemens Först (PhD Student, Clausthal University of Technology and Vienna University of Technology, Austria)
2001-2004	Johannes Kästner (Schimpl) (PhD Student, Clausthal University of Technology)

1997-2000	Hans Martin Senn (PhD student, Swiss Federal Institute of Technology, ETH Zurich, Switzerland).
1997	Prof. Helena Petrilli (Professor on sabbatical, University of Sao Paolo, Brazil.)
1994-1997	Ernst Nusterer (PhD student, Vienna University of Technology, Austria).
1992-1994	Peter Margl (PhD student, Vienna University of Technology, Austria).
1993	Paolo Carloni (PhD student, University of Florence, Italy.)
1992	Johannes Sarnthein (PhD student, Vienna University of Technology, Austria).
1991-1992	Dr. Andrew J. Fisher (Post-Doc, on leave from University of Oxford, UK).

Diploma, Bachelor and Master students

2021-03.2022	Patrick Kaiser (Master Student Chemistry, Clausthal University of Technology)
7.2021	Lukas Rump (Master, Physics, Göttingen University)
5.2019	Ingolf Harden, (Master, Chemistry, Clausthal University of Technology)
12.2017	Michael Ten Brink, (Master, Physics, Göttingen University)
11.2017	Heike Eisenlohr, (Master, Physics, Göttingen University)
4.2016	Ingolf Harden, (Bachelor, Chemistry, Clausthal University of Technology)
1.2014	Philipp Seichter, (Bachelor, Chemistry, Clausthal University of Technology)
11.2012	Robert Schade, (Master, Physics, Georg August University, Göttingen)
9.2015	Loay Abdelhafiz Elalfy (Master, Physics, Göttingen University)
1.2012	Jennifer Mohr, (Diploma Physics, Clausthal University of Technology)
11.2012	Christian Rößler (Diploma, Physics, Clausthal University of Technology
6.2011	Rolf Fader, (Diploma, Physics, Clausthal University of Technology)
7.2010	Oskar Stangenberg, (Bachelor, Physics, Clausthal University of Technology)

1.2009	Daniel Grieger, (Diploma, Physics, Clausthal University of Technology)
11.2007	Sineng Sun, (Diploma, Physics, Clausthal University of Technology)
	Holger Federmann, (Diploma, Physics, Clausthal University of Technology)
7.2008	Emanuel Hoffmann, (Diploma Physics, Clausthal University of Technology)
10.2006	Christian Walther (Diploma Physics, Clausthal University of Technology)
2004-??	Alexander Poddey (Diploma Physics, Clausthal University of Technology)
2005-6.2006	David Reibold (Diploma Student, Clausthal University of Technology)
2005-??	Manuel Kremer (Diploma Student, Clausthal University of Technology)
-11.2004	Sascha Hemmen (Diploma Physics, Clausthal University of Technology)
2002-2003	Sven Müller (Diploma Student, Clausthal University of Technology)
2002-2003	Mike Thieme (Diploma Student, Clausthal University of Technology)

Teaching

Bachelor in Physics

- Theoretical Physics I: Classical Mechanics (4V2Ü)
- Theoretical Physics II: Electrodynamics (4V2Ü)
- Theoretical Physics III: Quantum Physics (4V2Ü)
- Theoretical Physics IV: Statistical Physics (4V2Ü)

Master in Physics

- Advanced Topics of Theoretical Physics I: Introduction to Solid-State Theory (4V/2Ü)
- Advanced Topics of Theoretical Physics II: Advanced Solid-State Theory (4V/2Ü)
- Advanced Topics of Theoretical Physics III: The Statistical Properties of Matter (3V)
- Quantum Mechanics of the Chemical Bond: (3V/Ü)
- Hands-on Course on ab-initio Calculations. (two-week Block course, 80 hours.)
  - Theory of ab-initio calculations (lecture)
  - Electronic structure made simple (lecture)
  - Hands on course with the CP-PAW code (practice sessions)

Patents

[1] **"Structure especially a semi-conductor structure, in addition to a method for the production of said structure**: C.J. Först, C. Ashman, and P.E. Blöchl *German patent* **DE10303875B4** (Mar. 16, 2006).

[2] **Processing of Textual Information and Automated Apprehension of Information**: G.K. Binnig, P.E. Blöchl, and J. Klenk *United States Patent* **US6871199B1** (Mar. 22, 2005).

[3] **File or Database Manager Systems Based On a Fractal Hierarchical Structure**: G.K Binnig, P.E. Blöchl, and J. Klenk *United States Patent* **US6792418B1** (Sept. 14, 2004).

[4] **Method for Fabricating SiON Waveguides**: R. Beyeler, P.Blöchl, G.L. Bona, R.W. German, F. Horst, B.J. Offrein, H.L. Salemink, and D.W. Wiessmann *European Patent* **EP1261554B1** (Oct. 20, 2004).

[5] **Signal Processing by Means of Resonators**: P.E. Blöchl, U. Dürig, and O. Folini *United States Patent* **US6791433B1** (Sep. 14, 2004).

[6] **Optical Waveguide Device**: P.E. Blöchl, G. Bona, R. Germann, F. Horst, I. Massarek, B.J. Offrein, and H.W.M. Salemink *United States Patent* **US6678452B1** (Jan. 13, 2004).

[7] **Magnetic Sensing of Motion in Microfabricated Devices**: P.E. Blöchl, C. Rossel, and M. Willemin *United States Patent* **US6611140B1** (Aug. 26, 2003).

[8] **Optical Device with a Defined Total Stress and Method for Manufacturing it**: P.E. Blöchl, G. Bona, R. Germann, F. Horst, I. Massarek, B.J. Offrein, H.W.M. Salemink, and D. Wiesmann *United States Patent* **US6501895B1** (Dec. 31, 2002).

Publications

[1] **A critical View on e_g Occupancy as a Descriptor for Oxygen Evolution Catalytic Activity in $LiMn_2O_4$ Nanoparticles**: Florian Schönewald, Marco Eckhoff, Max Baumung, Marcel Risch, Peter E. Blöchl, Jörg Behler, and Cynthia A. Volkert *arXiv* **2007.04217** (submitted 2020).

[2] **Real-time non-adiabatic dynamics in the one-dimensional Holstein model: Trajectory-based vs exact methods**: M. ten Brink, S. Gräber, M. Hopjan, D. Jansen, J. Stolpp, F. Heidrich-Meisner, and P. E. Blöchl *J. Chem. Phys.* **156**, 234109 (2022).

[3] **Hydrogen-related defects in titanium dioxide at the interface to palladium**: Mohsen Sotoudeh, Marian David Bongers-Loth, Vladimir Roddatis, Jakub Čížek, Carsten Nowak, Martin Wenderoth, Peter Blöchl, and Astrid Pundt *Phys. Rev. Materials* **5**, 125801 (2021).

[4] **Orbital-order phase transition in $Pr_{1-x}Ca_xMnO_3$ probed by photovoltaics**: B. Kressdorf, T. Meyer, M. ten Brink, C. Seick, S. Melles, N. Ottinger, T. Titze, H. Meer, A. Weisser, J. Hoffmann, S. Mathias, H. Ulrichs, D. Steil, M. Seibt, P. E. Blöchl, and C. Jooss *Phys. Rev. B* **103**, 235122 (2021).

[5] **A review of density functional models for the description of Fe(II)**: Anton Römer, Lukas Hasecke, Peter Blöchl, and Ricardo A. Mata *Molecules* **25**, 5176 (2020).

[6] **Ultrafast spin-nematic and ferroelectric phase transitions induced by femtosecond light pulses**: Sangeeta Rajpurohit, Liang Z. Tan, Christian Jooss, and P. E. Blöchl *Phys. Rev. B* **102**, 174430 (2020).

[7] **Predicting oxidation and spin states by high-dimensional neural networks: Applications to lithium manganese oxide spinels**: Marco Eckhoff, Knut Nikolas Lausch, Peter E. Blöchl, and Jörg Behler *J. Chem. Phys.* **153**(16), 164107 (2020).

[8] **Room-Temperature Hot-Polaron Photovoltaics in the Charge-Ordered State of a Layered Perovskite Oxide Heterojunction**: B. Kressdorf, T. Meyer, A. Belenchuk, O. Shapoval, M. ten Brink, S. Melles, U. Ross, J. Hoffmann, V. Moshnyaga, M. Seibt, P. Blöchl, and C. Jooss *Phys. Rev. Applied* **14**, 054006 Nov (2020).

[9] **Closing the Gap between Theory and Experiment for Lithium Manganese Oxide Spinels Using a High-Dimensional Neural Network Potential**: Marcel Risch Cynthia A. Volkert Peter E. Blöchl Jörg Behler Marco Eckhoff, Florian Schönewald *Phys. Rev. B.* **102**, 174102 (2020).

[10] **Dynamic observation of Mn-adatom mobility at perovskite oxide catalyst interfaces to water**: G. Lole, V. Roddatis, U. Ross, M. Risch, T. Meyer, L. Rump, J. Geppert, G. Wartner, P. Blöchl, and Ch. Jooss *Commun. Mater.* **1**, 68 (2020).

[11] **Evolution of the magnetic and polaronic order of** $Pr_{1/2}Ca_{1/2}MnO_3$ **following an ultrashort light pulse**: Sangeeta Rajpurohit, Christian Jooss, and Peter E. Blöchl *Phys. Rev. B* **102**, 014302 (2020).

[12] **Hybrid density functional theory benchmark study on lithium manganese oxides**: Marco Eckhoff, Peter E. Blöchl, and Jörg Behler *Phys. Rev. B* **101**, 205113 (2020).

[13] **Surface resonance of the (2x1) reconstructed lanthanum hexaboride (001)-cleavage plane: A combined STM and DFT study**: P. Buchsteiner, F. Sohn, J. G. Horstmann, J. Voigt, M. Ciomaga Hatnean, G. Balakrishnan, C. Ropers, P. E. Blöchl, and M. Wenderoth *Phys. Rev. B* **100**, 205407 (2019).

[14] **Density functional study of half-metallicity and spin polarization in** $\mathbf{Fe_{1-x}T_xS_2}$ **with T = Mn,Ni**: Abdesalem Houari and Peter E. Blöchl *J. Phys.: Condens. Matter* **30**, 305501 (2018).

[15] **Adaptive cluster approximation for reduced density-matrix functional theory**: Robert Schade and Peter E. Blöchl *Phys. Rev. B* **97**, 245131 (2018).

[16] **Relaxation of photoexcitations in polaron-induced magnetic microstructures**: O. Schumann F. R. A. Biebl M. Sotoudeh S. C. Kramer P. E. Blöchl S. Kehrein S. R. Manmana T. Köhler, S. Rajpurohit *Phys. Rev. B* **97**, 235120 (2018).

[17] **Reduced density-matrix functionals from many-particle theory**: Robert Schade, Ebad Kamil, and Peter E. Blöchl *Eur. Phys. J. Spec. Top.* **226**, 2677–2692 (2017).

[18] **Electronic structure of** $\mathbf{Pr_{1-x}Ca_xMnO_3}$: Mohsen Sotoudeh, Sangeeta Rajpurohit, Peter Blöchl, Daniel Mierwaldt, Jonas Norpoth, Vladimir Roddatis, Stephanie Mildner, Birte Kressdorf, Benedikt Ifland, and Christian Jooss *Physical Review B* **95**, 235150 (2017).

[19] **Evolution of Hot Polaron States with a Nanosecond Lifetime in a Manganite Perovskite**: Dirk Raiser, Stephanie Mildner, Benedikt Ifland, Mohsen Sotoudeh, Peter Blöchl, Simone Techert, and Christian Jooss *Advanced Energy Materials* **7**(12), 1602174 (2017) 1602174.

[20] **Reduced density-matrix functionals applied to the Hubbard dimer**: Ebad Kamil, Robert Schade, Thomas Pruschke, and Peter E. Blöchl *Physical Review B* **93**, 085141 (2016).

[21] **Beam Matching: a method to study transport accross multiple interfaces**: D. Basu and P.E. Blöchl *Physica status solidi A* **213**, 635 (2015).

[22] **Temperature and doping dependent optical absorption in the small polaron system $\mathbf{Pr_{1-x}Ca_xMnO_3}$**: S. Mildner, J. Hoffmann, C. Jooss, P. E. Blöchl, and S. Techert *Physical Review B* **92**, 35145 (2015).

[23] **Density-matrix functionals from Green's functions**: Th. Pruschke P.E. Blöchl and M. Potthoff *Physical Review B* **88**, 205139 (2013).

[24] **In-situ Electrochemical Microscopy Study of Oxygen Evolution Activity of Doped Manganite Perovskites**: S. Raabe, D. Mierwaldt, J. Ciston, M. Uijttewaal, H. Stein, J. Hoffmann, Y. Zhu, P. Blöchl, and Ch. Jooss *Adv. Functional Materials* **22**, 3378 (2012).

[25] **Node-less atomic wave functions, Pauli repulsion and systematic projector augmentation**: P.E. Blöchl and C. Först *Arxiv* (1210.5937) (2012).

[26] **Method to Include Explicit Correlations into Density-Functional Calculations based on Density-Matrix Functional Theory**: P. E. Blöchl, C. F. J. Walther, and Th. Pruschke *Phys. Rev. B* **84**, 205101 (2011).

[27] ***Theory and Practice of Density functional theory*** in The LDA+DMFT Approach to Strongly Correlated Materials : volume 1 of Modelling and Simulation Forschungszentrum Jülich GmbH, Institute for Advanced Simulations P. E. Blöchl (2011).

[28] **Dynamical Dimer Method for the Determination of Transition States with *Ab-Initio* Molecular Dynamics**: A. Poddey and P.E. Blöchl *J. Chem. Phys.* **128**, 44107 (2008).

[29] **Ammonia Production at the FeMo-Cofactor of Nitrogenase: Results from Density-Functional Theory**: J. Kästner and P.E. Blöchl *J. Am. Chem. Soc.* **129**, 2998 (2007).

[30] **Molecular Design of Interfaces based on Density-Functional Simulations**: P.E. Blöchl, C.J. Först, C.R. Ashman, K. Schwarz, and A. Reyes Huamantinco *Z. Anorg. Allg. Chem.* **632**, 2075 (2006).

[31] **Band Alignment at the $\mathbf{La_2Hf_2O_7}$/(001)Si Interface**: G. Seguini, S. Spiga, E. Bonera, M. Fanciulli, A. Reyes Huamantinco, C.J. Först, C.R. Ashman, P.E. Blöchl, A. Dimoulas, and G. Mavrou *Applied Physics Letters* **88**, 202903 (2006).

[32] ***Modeling of Growth of High-k Oxides on Semiconductors*** in Advanced Gate Stacks on High Mobility Semiconductors : volume 27 of Springer Series for Advanced Microelectronics Springer Verlag C.J. Först, C.R. Ashman, K. Schwarz, and P.E. Blöchl (2007).

[33] **Structural and Electronic Properties of the Interface between the High-k Oxide LaAlO3 and Si(001)**: C.J. Först, K. Schwarz, and P.E. Blöchl *Phys. Rev. Lett.* **95**, 137602 (2005).

[34] **Activation and Protonation of Dinitrogen at the FeMo-Cofactor of Nitrogenase**: J. Kästner, S. Hemmen, and P.E. Blöchl *J. Chem. Phys.* **123**, 74306 (2005).

[35] **Towards Understanding the Workings of Nitrogenase from DFT Calculations**: J. Kästner and P.E. Blöchl *ChemPhysChem* **6**, 1724 (2005).

[36] **Mit dem Computer in die Nanowelt: Ab-initio Simulations von der Biochemie zur Halbleitertechnologie,**: P.E. Blöchl *Jahrbuch 2004 der Braunschweigischen Wissenschaftl. Gesellschaft*, 59 (2005).

[37] **Ab-initio Simulations on Growth and Interface Properties of Epitaxial High-k Oxides on Silicon,**: C.J. Först, C.R. Ashman, K. Schwarz, and P.E. Blöchl *Microelectronic Engineering* **80**, 402 (2005).

[38] **A Model for Acetylene Reduction by Nitrogenase derived from Density Functional Theory**: J. Kästner and P.E. Blöchl *Inorg. Chem.* **44**, 4568 (2005).

[39] ***Electronic structure methods: Augmented Waves, Pseudopotentials and the Projector Augmented Wave method*** in Handbook of Materials Modeling : volume 1 Springer P.E. Blöchl, C.J. Först, and J. Kästner (2005).

[40] **Interaction of NaCl with solid water**: A. Borodin, O. Höfft, U. Kahnert, V. Kempter, A. Poddey, and P.E. Blöchl *J. Chem. Phys.* **121**, 9671 (2004).

[41] **Chemistry of La on the Si(001) surface from first principles**: C.R. Ashman, C.J. Först, K. Schwarz, and P.E. Blöchl *Phys. Rev. B* **70**, 155330 (2004).

[42] **First-principles Calculations of Strontium on Si(001)**: C.R. Ashman, C.J. Först, K. Schwarz, and P.E. Blöchl *Phys. Rev. B* **69**, 75309 (2004).

[43] * **The Interface between Silicon and a High-K Oxide**: C.J. Först, C.R. Ashman, K. Schwarz, and P.E. Blöchl *Nature* **53**, 427 (2004).

[44] **Nitrogen Binding to the FeMo Cofactor of Nitrogenase**: J. Schimpl, H.M. Petrilli, and P.E. Blöchl *J. Am. Chem. Soc.* **125**, 15772–15778 (2003).

[45] **Ab-initio Molecular Dynamics with a Continuum Solvation Model**: H.M. Senn, P.M. Margl, R. Schmid, T. Ziegler, and P.E. Blöchl *J. Chem. Phys.* **118**, 1089–1100 (2003).

[46] * **Implementation of an all-electron GW approximation based on the Projector Augmented Wave Method without Plasmon Pole Approximation: Application to Si, SiC, AlAs, InAs, NaH, and KH**: S. Lebegue, B. Arnaud, M. Alouani, and P.E. Blöchl *Phys. Rev. B* **67**, 155208 (2003).

[47] *The Projector Augmented Wave Method: Ab-initio Molecular Dynamics Simulations with Full Wave Functions: P.E. Blöchl, C. Först, and J. Schimpl *Bull. Mater. Sci.* **26**, 33 (2003).

[48] **Heteroepitaxial Growth of High-K Oxides: Insights from First-Principles Calculations on Zr on Si(001)**: C.J. Först, P.E. Blöchl, and K. Schwarz *Comp. Mat. Sci.* **27**, 70–74 (2003).

[49] **Second Generation Wave Function Thermostat for Ab-initio Molecular Dynamics**: P.E. Blöchl *Phys. Rev. B.* **65**, 104303 (2002).

[50] **LDA+U Calculated Electronic and Structural Properties of NiO(001) and NiO(111) p(2x2) Surfaces**: O. Bengone, M. Alouani, J. Hugel, and P.E. Blöchl *Comp. Mater. Sci.* **24**, 192–198 (2002).

[51] **A Car-Parrinello Study of the Formation of Oxidizing Intermediates from Fenton's Reagent in Aqueous Solution**: B. Ensing, F. Buda, P.E. Blöchl, and E.J. Baerends *Phys. Chem. Chem. Phys.* **4**, 3619 (2002).

[52] **Chemical Involvement of Solvent Water Molecules in Elementary Steps of the Fenton Chemistry**: B. Ensing, F. Buda, P.E. Blöchl, and E.J. Baerends *Angew. Chem.* **113**, 2977 (2001) Angew. Chem. Int. Ed. Engl. **40**, 2893 (2001)).

[53] **Solvation Effects on the S_N2 Reaction between CH_3Cl and Cl^- in Water**: B. Ensing, E.J. Meyer, P.E. Blöchl, and E.J. Baerends *J. Phys. Chem. A* **105**, 3300 (2001).

[54] **Replacement of Forming Gas Anneal by an Applied Voltage**: P.E. Blöchl and G.L. Bona *Research Disclosure* **446**, 664 (2001).

[55] **Low Loss, Deuterium-Diffused SiON Material for Planar Optical Waveguide Circuits (SioN:D)**: P.E. Blöchl and H. Salemink *Research Disclosure* **444**, 666 (2001).

[56] **Delaying Breakdown of Gate Oxides by Reverting the Electric Field in the Oxide**: P.E. Blöchl and G.L. Bona *Research Disclosure* **444**, 666 (2001).

[57] * **Implementation of the Projector Augmented Wave LDA+U Method: Application to the Electronic Structure of NiO**: O. Bengone, M. Alouani, P.E. Blöchl, and J. Hugel *Phys. Rev. B* **62**, 16392 (2000).

[58] **Towards Solvation Simulations with a Combined Ab-Initio Molecular Dynamics and Molecular Mechanics Approach**: T.K. Woo, P.E. Blöchl, and T. Ziegler *J. Mol. Struc. (THEOCHEM)* **506**, 313–344 (2000).

[59] ***Defects in Silica Related to Breakdown in Gate Oxides*** in Proc. 3rd Japan-Korea Joint Workshop on First-Principles Electronic Structure Calculations : P.E. Blöchl.

[60] * **Towards an Alkene Hydroamination Catalyst: Static and Ab-Initio DFT Studies**: H.M. Senn, P.E. Blöchl, and A. Togni *J. Amer. Chem. Soc.* **122**, 4098 (2000).

[61] * **First-Principles Calculations of Defects in Oxygen-Deficient Silica Exposed to Hydrogen**: P.E. Blöchl *Phys. Rev. B* **62**, 6158 (2000).

[62] **Fractal Network N-ter Order for Handling Complex Structures**: M. Athelogou, M. Baats, G.K Binnig, P.E. Blöchl, A. Kharadi, J. Klenk, and G. Schmidt *PCT Publication WO 00/20946* ((April 13, 2000)).

[63] **Monomer Capture in Brookhart's Ni(II) Diimine Olefin Polymerization Catalyst: Static and Dynamic Quantum Mechanics/Molecular Mechanics Study**: T.K. Woo, P.E. Blöchl, and T. Ziegler *J. Phys. Chem. A* **104**, 121 (2000).

[64] **Phosphane Lone-Pair Energies as a Measure of Ligand Donor Strengths and Relation to Activation Energies**: H.M. Senn, D.V. Deubel, P.E. Blöchl, A. Togni, and G. Frenking *Journal of Molecular Structure: THEOCHEM* **506**, 233–242 (2000).

[65] **Taming the Ground-State and Optical Properties of Transition-Metal Oxides**: O. Bengone, M. Alouani, J. Hugel, and P.E. Blöchl *Comp. Mater. Sci.* **17**, 146–155 (2000).

[66] * **Hydrogen Electrochemistry and Stress-Induced Leakage Current in Silica**: P.E. Blöchl and J.H. Stathis *Phys. Rev. Lett.* **83**, 372 (1999).

[67] **Aspects of Defects in Silica Related to Dielectric Breakdown of Gate Oxides in MOSFET**: P.E. Blöchl and J.H. Stathis *Physica B* **273-274**, 1022–1026 (1999).

[68] **First-Principles Molecular Dynamics Study of Small Molecules in Zeolites**: K. Schwarz, E. Nusterer, and P.E. Blöchl *Catalysis Today* **50**, 501–509 (1999).

[69] **Molecular Reaction Modeling from Ab-Initio Molecular Dynamics**: In D.G. Truhlar and K. Morokuma, editors, *Transition State Modeling for Catalysis*, page 88. American Chemical Society (1999) P.E. Blöchl, H.M. Senn, and A. Togni.

[70] **Material with Reduced Optical Absorption**: P.E. Blöchl, R. Germann, I. Massarek, B.J. Offrein, and H.W.M. Salemink *PCT Publication* **WO 99/44937** ((Sep. 10, 1999)) European Patent Application Nr. 98103888.8 (Mar. 4, 1998).

[71] **Evidence for a Stable Ti(IV) Metallocene Dihydrogen Complex from Ab-Initio Molecular Dynamics.**: T.K. Woo, P.M. Margl, P.E. Blöchl, and T. Ziegler *J. Am. Chem. Soc.* **120**, 2174 (1998).

[72] * **Electric Field Gradient Calculations using the Projector Augmented Wave Method**: H.M. Petrilli, P.E. Blöchl, P. Blaha, and K. Schwarz *Phys. Rev. B* **57**, 14690 (1998).

[73] **Ab-Initio Calculation of Binding and Diffusion of a Ga Adatom on the GaAs(001)-c(4×4) Surface**: J.G. LePage, M. Alouani, D.L.Dorsey, J.W. Wilkins, and P.E. Blöchl *Phys. Rev. B* **58**, 1499 (1998).

[74] **First-Principles Investigations of a "quasi-one dimensional" Charge-Transfer Molecular Crystal: TTF-2,5Cl2BQ**: C. Katan, C. Koenig, and P.E. Blöchl *Comp. Mater. Sci.* **10**, 325–329 (1998).

[75] **A Combined Car-Parrinello QM/MM Implementation for *ab-initio* Molecular Dynamics Simulations of Extended Systems: Application to Transition Metal Catalysts**: T.K. Woo, P.M. Margl, P.E. Blöchl, and T. Ziegler *J. Phys. Chem. B* **101**, 7877 (1997).

[76] * **Static and ab-initio Dynamics Study of the Titanium (IV) Constrained Geometry Catalyst ($CpSiH_2NH$) Ti-R^+: 2. Chain Termination and Long Chain Branching**: T.K. Woo, P. Margl, T. Ziegler, and P.E. Blöchl *Organometallics* **16**, 3454 (1997).

[77] **Hydrocarbon Adsorption on Si(001): When Does the Si Dimer Bond Break?**: A.J. Fisher, P.E. Blöchl, and G.A.D. Briggs *Surf. Sci.* **374**, 298–305 (1997).

[78] **Ab initio Molecular Dynamics Calculations to Study Catalysis**: K. Schwarz, E. Nusterer, P. Margl, and P.E. Blöchl *Int. J. Quantum Chem.* **61**, 369 (1997).

[79] **Ab initio Calculations of One–Dimensional Band Structures of Mixed–Stack Molecular Crystals**: C. Katan, C. Koenig, and P.E. Blöchl *Solid State Comm.* **102**, 589–594 (1997).

[80] **Electronic Structure Calculations and Molecular Dynamics Simulations of Mixed–Stack Charge–Transfer Complexes**: C. Katan, C. Koenig, and P.E. Blöchl *Bull. of the Inst. of Phys. and Theoretical Chemistry (Biuletyn Inst. Chemii Fizycznej i Teoretycznej Politechniki Wroclawskiej* **4** (1997).

[81] **Die Methode der Projektoraugmentierten Wellen**: P.E.Blöchl *Habilitationsschrift, Vienna University of Technology* (1996).

[82] **Structure and Dynamics of Methanol in a Zeolite**: E. Nusterer, P.E. Blöchl, and K. Schwarz *Angew. Chem.* **108**, 187–189 (1996) (Angew. Chem. Int. Ed. Engl. 35,(2), 175-177 (1996)).

[83] * **Combined Static and Dynamic Density Functional Study of the Ti(IV) Constrained Geometry Catalyst ($CpSiH_2NH$)TiR^+. 1. Resting States and Chain Propagation**: T.K. Woo, P.M. Margl, J.C.W. Lohrenz, P.E. Blöchl, and T. Ziegler *J. Am. Chem. Soc.* **118**, 13021–13030 (1996).

[84] * **A Dynamical Density Functional Study on the Reaction of Ethylene with $Cp_2Zr(C_2H_5)^+$**: P. Margl, J.C.W. Lohrenz, T. Ziegler, and P.E. Blöchl *J. Am. Chem. Soc.* **118**, 4434–4441 (1996).

[85] **Migratory CO Insertion and Aldehyde Formation in Carbonylation of Methane by the $Rh(PH_3)_2Cl$ Catalyst. A Dynamical Density Functional Study**: P. Margl, T. Ziegler, and P.E. Blöchl *J. Am. Chem. Soc.* **118**, 5412–5419 (1996).

[86] **Ab initio Molecular-Dynamics Study of Diffusion and Defects in Solid Li_3N**: J. Sarnthein, K. Schwarz, and P.E. Blöchl *Phys. Rev. B* **53**, 9084–9091 (1996).

[87] **First-Principles Molecular-Dynamics Simulations for Neutral *p*-Chloranil and its Radical Anion**: C. Katan, P.E. Blöchl, P. Margl, and C. Koenig *Phys. Rev. B* **53**, 12112–12120 (1996).

[88] * **First Principles Investigation of Enantioselective Catalysis: Asymmetric Allylic Amination with Pd Complexes Bearing P,N-Ligands**: P.E. Blöchl and A. Togni *Organometallics* **15**, 4125–4132 (1996).

[89] **Interaction of Water and Methanol with a Zeolite at High Coverages**: E. Nusterer, P.E. Blöchl, and K. Schwarz *Chem. Phys. Lett.* **253**, 448–455 (1996).

[90] **Ab-initio Molecular Dynamics with the Projector Augmented Wave Method**: In B.B. Laird, R.B. Ross, and T. Ziegler, editors, *Chemical Applications of Density-Functional Theory*, pages 54–69. American Chemical Society (1996) P.E. Blöchl, P. Margl, and K. Schwarz.

[91] **Reaction of Methane with $Rh(PH_3)_2Cl$: A Dynamical Density Functional Study**: P. Margl, T. Ziegler, and P.E. Blöchl *J. Am. Chem. Soc.* **117**, 12625–12634 (1995).

[92] * **Electrostatic Decoupling of Periodic Images of Plane-Wave-Expanded Densities and Derived Atomic Point Charges**: P.E. Blöchl *J. Chem. Phys* **103**, 7422–7428 (1995).

[93] **Electronic Structure of Cu, Zn Superoxide Dismutase Active Site and Its Interaction with the Substrate**: P. Carloni, P.E. Blöchl, and M. Parrinello *J.Phys. Chem.* **99**, 1339–1348 (1995).

[94] **Dynamics of Beryllocene**: P. Margl, K. Schwarz, and P.E. Blöchl *J. Chem. Phys.* **103**, 683–690 (1995).

[95] **Electronic Structure of Crystalline $(NH_4)_2CuCl_4$ from First Principles**: P. Carloni, P.E. Blöchl, and P.L. Orioli *Gazzetta Chimica Italiana* **125**, 497–500 (1995).

[96] **Fluxional Dynamics of Beryllocene**: P. Margl, K. Schwarz, and P.E. Blöchl *J. Am. Chem. Soc.* **116**, 11177–11178 (1994).

[97] **Finite-Temperature Characterization of Ferrocene from First-Principles Molecular Dynamics Simulations**: P. Margl, K. Schwarz, and P.E. Blöchl *J. Chem. Phys.* **100**, 8194–8203 (1994).

[98] ** **Projector Augmented-Wave Method**: P.E. Blöchl *Phys. Rev. B* **50**, 17953–17979 (1994).

[99] ** **Improved Tetrahedron Method for Brillouin-Zone Integrations**: P.E. Blöchl, O. Jepsen, and O.K. Andersen *Phys. Rev. B* **49**, 16223–16233 (1994).

[100] **Hypothetical Carbon Modifications Derived from Zeolite Frameworks**: R. Nesper, K. Vogel, and P.E. Blöchl *Angew. Chem.* **105**, 786–788 (1993) (Angew. Chem. Int. Ed. English 32(5), 701-703 (1993)).

[101] * **First-Principles Calculations of Self-Diffusion Constants in Silicon**: P.E. Blöchl, E. Smargiassi, R. Car, D.B. Laks, W. Andreoni, and S.T. Pantelides *Phys. Rev. Lett.* **70**, 2435–2438 (1993).

[102] * **Adsorption and Scanning-Tunneling-Microscope Imaging of Benzene on Graphite and MoS_2**: A.J. Fisher and P.E. Blöchl *Phys. Rev. Lett.* **70**, 3263–3266 (1993).

[103] ** **Crystal Orbital Hamilton Populations (COHP). Energy-Resolved Visualization of Chemical Bonding in Solids Based on Density-Functional Calculations**: R. Dronskowski and P.E. Blöchl *J. Phys. Chem.* **97**, 8617–8624 (1993).

[104] * **First-Principles Calculations of Hyperfine Parameters**: C.G. Van de Walle and P. Blöchl *Phys. Rev. B* **47**, 4244–4255 (1993).

[105] ***First-Principles Calculations of Organometallic Compounds*** in Proc. NATO ARW *Computations for the Nano-Scale* : volume 240 of E: Applied Sciences Kluwer, Dordrecht P. Margl, K. Schwarz, and P.E. Blöchl (1993).

[106] ***Adsorption and STM Imaging of Organic Molecules from First Principles*** in Proc. NATO ARW *Computations for the Nano-ScaleAdsorption and STM Imaging of Organic Molecules from First Principles* : volume 240 of E: Applied Sciences Kluwer, Dordrecht A.J. Fisher and P.E. Blöchl (1993).

[107] * **Adiabaticity in First-Principles Molecular Dynamics**: P.E. Blöchl and M. Parrinello *Phys. Rev. B* **45**, 9413–9416 (1992).

[108] * **Native Defects and Self-Compensation in ZnSe**: D.B. Laks, C.G. Van de Walle, G.F. Neumark, P.E. Blöchl, and S.T. Pantelides *Phys. Rev. B* **45**, 10965–10978 (1992).

[109] **Interacting Loop-Current Model of Superconducting Networks**: C.C. Chi, P. Santhanam, and P.E. Blöchl *J. Low Temp. Phys.* **88**, 163–195 (1992).

[110] **Ab-Initio Molecular Dynamics of Semiconductor Defects**: R. Car, P.E. Blöchl, and E. Smargiassi *Materials Science Forum* **83-87**, 433–446 (1992).

[111] **Simulation im Nanometerbereich**: P. Blöchl *Schw. Techn. Zeitschr.* **12**, 10–16 (1992).

[112] ***First Principles Calculations of Diffusion Constants in Silicon*** in Proc. Second Int. Symp. on Process Physics and Modeling in Semiconductor Technology : volume 91 Electrochemical Society, Incorporated P.E. Blöchl, C.G. Van de Walle, and S.T. Pantelides (1991).

[113] **Novel Semiconductors and Intermetallic Compounds – In Search of New Materials**: K.H. Vogel, R. Nesper, P.E. Blöchl, and M. Parrinello *C^4 Bulletin 4* (1991).

[114] **First-Principles Calculations of Diffusion Coefficients: Hydrogen in Silicon**: P.E. Blöchl, C.G. Van de Walle, and S.T. Pantelides *Phys. Rev. Lett.* **64**, 1401–1404 (1990).

[115] **Exchange Correlation Potentials in Schottky Barriers and Heterojunctions**: G.P. Das, P.E. Blöchl, O.K. Andersen, N.E. Christensen, and O. Gunnarson *Phys. Rev. Lett.* **65**, 2083–2084 (1990).

[116] * **Generalized Separable Potentials for Electronic-Structure Calculations**: P.E. Blöchl *Phys. Rev. B* **41**, 5414 (1990).

[117] **Phase Boundaries of Superconducting Networks: A New Approximation Scheme**: C.C. Chi, P. Santhanam, and P.E. Blöchl *Phys. Rev. B* **42**, 76–79 (1990).

[118] **Electronic Structure of Ordered and Disordered Pd_3Fe**: S.K. Bose, J. Kudrnovsky, M. van Schilfgaarde, P.E. Blöchl, O. Jepsen, M. Methfessel, A.T. Paxton, and O.K. Andersen *J. Magn. Mat.* **87**, 97–105 (1990).

[119] ***Electronic Structure of a Metal-Ceramic Interface: Ab Initio Calculations for MgO/Ag*** in Proc. Int. Workshop *Metal-Ceramic Interfaces* : Acta Metallurgica Inc. P. Blöchl, G.P. Das, H.F. Fischmeister, and U. Schönberger (1990).

[120] *First-Principles Calculations of Self-Diffusion Coefficients in Silicon* in **Proc. 20th Int. Conf. on the Physics of Semiconductors** : World Scientific, Singapore P.E. Blöchl, D.B. Laks, S.T. Pantelides, E. Smargiassi, R. Car, W. Andreoni, and M. Parrinello (1990).

[121] **Gesamtenergien, Kräfte und Metall-Halbleiter Grenzflächen** P. Blöchl PhD thesis University of Stuttgart (1989).

[122] * **Electronic Structure and Schottky-Barrier Heights of (111) $NiSi_2$/Si A- and B-Type Interfaces**: G.P. Das, P.E. Blöchl, O.K. Andersen, N.E. Christensen, and O. Gunnarson *Phys. Rev. Lett.* **63**, 1168–1171 (1989).

[123] ***Total Energy and Force Calculations with the LMTO Method*** in Proc. Int. Symp. on Atomistic Simulation of Materials: Beyond Pair Potentials : Plenum Press New York O.K. Andersen, M. Methfessel, C.O. Rodriguez, P. Blöchl, and H.M. Polatoglou (1989).

[124] ***Calculated Electronic Structures and Schottky Barrier Heights of (111) $NiSi_2$/Si A- and B-Type Interfaces*** in Proc. NATO Advanced Research Workshop on *Metallization and Metal–Semiconductor Interfaces* : Plenum Press New York G.P. Das, P. Blöchl, N.E. Christensen, and O.K. Andersen (1989).

[125] ***Electronic Structure of Metal-Semiconductor Interfaces*** in Proc. 18th Annual Int. Symp. on Electronic Structure of Metals and Alloys : Gaussig G.P. Das, P.E. Blöchl, N.E. Christensen, and O.K. Andersen (1988).

[126] **Electronic Structure and Properties of $NiSi_2$ and $CoSi_2$ in the Flourite and Adamantane Structures**: W.R.L. Lambrecht, N.E. Christensen, and P.E. Blöchl *Phys. Rev. B* **36**, 2493–2503 (1987).

[127] ***First-Principles Tight-Binding Electronic Structure Calculations on Point Defects in Solids*** in Proc. 17th Annual Int. Symp. on Electronic Structure of Metals and Alloys : Gaussig M. Sob, O. Jepsen, O.K. Andersen, F. Beeler, and P.E. Blöchl (1987).

* Publications cited more than 100 times are marked by a star. Publications cited more than 1000 times are marked by two stars.

Three publications [98, 99, 103] have each been cited more than 1000 times and 23 papers have been cited more than 100 times. The total number of citations is about 60345 (Researcher ID B-3448-2012 of Dec. 10, 2021). The h-index is 44, that is 44 publications have been cited at least 44 times. The list contains, among others, one Nature article [43], seven Physical Review Letters[33, 66, 101, 102, 114, 115, 122], three Angewandte Chemie [52, 82, 100], nine publications in the Journal of the American Chemical Society [29, 44, 60, 71, 83, 84, 85, 91, 96] and thirty-one Physical Review B[4, 6, 9, 11, 12, 13, 15, 16, 18, 20, 22, 23, 26, 41, 42, 46, 49, 57, 61, 72, 73, 86, 87, 98, 99, 104, 107, 108, 116, 117, 126].

Invited Conference Presentations

1. **"Towards simple ab-initio calculations of strongly correlated materials"** Festkörpertag Südniedersachsten, Hanover, Germany; July 23, 2014

2. **"Linking the Greens function world to that of ground state functionals."** Quantum Theory of Solids (QTS-6), Aahrhus, Denmark; June, 24-26, 2014

3. **"Ground state correlations in DFT via density-matrix functional theory"** International Symposium on *"Recent Electronic-Structure Theories and Related Experiments"*, Stuttgart, Germany; Jun. 12-15, 2013

4. **"Density-matrix functional theory as bridge between DFT and explicit many-particle theory"** Second PIRE workshop: *"Graduate education in petascale many body methods for complex correlated systems"*, Göttingen, Germany; Jan 6-7, 2012

5. **"Theory and practice of density-functional theory"** Autumn School Hands-on LDA+DMFT, Forschungszentrum Jülich, Germany; Oct. 4-7, 2011

6. **"Density-matrix functional theory as bridge between DFT and explicit many-particle theory"** International CECAM Workshop *"Perspectives and challenges of many-particle methods"*, Bremen Center for Computational Materials Science, University of Bremen, Germany; Sept. 19-23, 2011

7. **"Strategies for solving Kohn Sham equations"** International Summer School on *"Electronic structure theory and materials design"*, Technical University of Denmark, Lyngby, Denmark; Aug 14-20, 2010

8. **"Projector-augmented wave implementation"** International Summer School on *"Electronic structure theory and materials design"*, Technical University of Denmark, Lyngby, Denmark; Aug 14-20, 2010

9. **"The workings of nitrogenase and new developments of the projector augmented wave method"** 238th American Chemical Society National Meeting, Washington DC, USA; Aug. 16-20, 2009

10. **"How nature breaks the strongest bond: The workings of nitrogenase"** Scientific Symposium Honoring Sok Pantelides *"Recent Advances in Materials Physics"*, Vanderbilt University, Nashville, Tennessee, USA; April 3-5, 2009

11. **"Molecular design of interfaces with Density-Functional Theory"** Südniedersächsischer Festkörpertag 2008, Hannover, Germany; June 13, 2008

12. **"Interfacing oxides and semiconductors: lessons from first-principles simulations"** IBM MRC Oxide Workshop; IBM Zurich Research Laboratory, Rüschlikon, Switzerland; Feb. 7-10, 2007

13. **"Molekulares Design von Grenzflächen auf der Basis von Dichtefunktionalsimulationen (Molecular design of interfaces based on density-functional theory)"** "Modellierung in der Festkörper und Materialchemie", 13. Vortragstagung of the GdCH, Aachen, Germany; Sept. 20-22,2006

14. **"First-principles calculations on the formation of epitaxial semiconductor oxide interfaces for future transistor generations"** Workshop *"Microelectronics meets catalysis"*, Delmenhorst, Germany; July 20-21, 2006

15. **"Insights on the nitrogen fixation mechanism from first principles"** PSII Tagung des SFB498, *"Protein-Cofactor Interaction"*, Berlin, Germany; May 5-6,2006

16. **"Analysis and design of materials-processes for future transistors"** *"DFTEM 2006 - bringing together two communities, International Conference on Density Functional Theory (DFT) and Transmission Electron Microscopy (TEM)"*, Vienna, Austria; Apr. 21-23, 2006

17. **"First-principles calculations on the formation of epitaxial semiconductor oxide interfaces for future transistor generations"** Computational Science Workshop 2006 (CSW2006), Tsukuba, Japan; Apr. 17-19, 2006

18. **"Towards computational materials design of oxide films"** Workshop on *"Ab-initio description of iron and steel (ADIS-2006)"*, Schloss Ringberg Castle, Tegernsee, Germany; Feb. 19-24, 2006

19. **"Insights on the formation of epitaxial high-K oxides on silicon from first principles"** MRS 2005 Fall Meeting, Boston, USA; Nov. 28-Dec.2, 2005

20. **"Hydrogen-related chemistry in silicon dioxide"** Workshop on *"Modeling materials in extreme environment"*, Washington D.C., USA; Sept. 24-25, 2005

21. **"The workings of the enzyme nitrogenase"** CPMD2005, Ascona, Switzerland; Sept. 3-8, 2005

22. **"Ab-initio simulations on growth and interface properties of high-k oxides on silicon"** *"INFOS (Insulating thin films on semiconductors)"*, Leuven, Belgium; June 22-24, 2005

23. **"How nature breaks the strongest bond – The workings of the enzyme nitrogenase"** *"PPES-III (Probing Potential Surfaces)"*, Zermatt, Switzerland; Apr. 3-8, 2005

24. **"Mit dem Computer in die Nanowelt: Ab-initio Simulationen von der Biochemie zur Halbleitertechnologie"** Plenarsitzung der Braunschweigischen Wissenschaftlichen Gesellschaft; Clausthal, Germany; Jul. 7, 2004

25. **"Enzymatic mechanism for biological nitrogen fixation from first principles; (Plenary talk)"** 18. Darmstädter Molecular Modeling Workshop; Erlangen, Germany; May 18-29, 2004

26. **"First-principles calculations of the formation of the $SrTiO_3$/Si interfaces"** 34th IEEE Semiconductor Interface Specialist Conference (SISC), Washington, DC, USA; Dec. 4-6, 2003

27. **"Ab-initio simulations on initial growth steps of high-K oxides on silicon: $SrTiO_3$/Si(001)"** MRS Fall Meeting 2003, Boston, MA, USA; Dec. 1-5, 2003

28. **"Tutorial on the PAW method"** Workshop on *"Application of density-functional theory in condensed-matter physics, Surface Physics,Chemistry, Engineering, and Biology"*, Fritz-Haber Institute, Berlin, Germany; July 21-30, 2003

29. **"Growth steps of $SrTiO_3$ on Si and band-offset Engineering by Controlled Oxidation"** Workshop on "Electronic structure of Condensed Matter II; Schloss Ringberg, Kreuth, Germany; June 22-24, 2003

30. **"Initial growth steps of high-k Oxides on silicon"** E-MRS Meeting, Strassbourg, France; June 10-13, 2003

31. **"Ab-initio calculations of degradation of Si/SiO2 and initial growth steps of high-k oxides on silicon"** March Meeting of the American Physical Society, Austin, TX, USA; Mar. 3-7, 2003.

32. **"Ab-initio simulation of growth of high-k oxides on silicon"** 3rd International Meeting *"Challenges in Predictive Process Simulation-ChiPPS 2002"*; Prague, Czech Republic ; Oct. 13-17, 2002 (Talk given by C.J. Först).

33. **"Tutorial on the projector augmented wave method"** Workshop on *"Realistic theories of correlated electron materials"*; Institute of Theoretical Physics, UCSB, Santa Barbara, CA, USA; Jul. 20-Dec.20, 2002 (i)

34. **"Ab-initio results from SiO_2 to high-k gate oxides"** Electronic Structure Workshop, Schloss Ringberg, Germany; Mai. 31-June 1, 2002

35. **"Ab-initio results from SiO_2 to high-k gate oxides"** Spring Meeting of the Material Research Society, San Francisco, CA, USA; Apr. 1-5, 2002

36. **"Insights on gate oxides in MOSFETs from first principles"** 42st Sanibel Symposium, St. Augustine, FL, USA; Feb. 23-Mar. 1, 2002

37. **"The Projector Augmented Wave method: algorithm and results"** 1st Conference of the Asian Consortium for Computational Materials Science, Bangalore, India; Nov. 28-30, 2001

38. **"A new two-thermostat formulation of ab-initio molecular dynamics"** 13th Annual Workshhop on Recent Developments in Electronic Structure Algorithms. Princeton, NJ, USA; Jun 15-18, 2001

39. **"Leakage currents amd breakdown in gate oxides of MOSFETs"** Symposium on *"Condensed matter theory"*; Max Planck Institute for Solid State Research, Stuttgart, Germany; May 23, 2001

40. **"Hydrogen electrochemistry in SiO_2 related to breakdown in gate oxides"** 41st Sanibel Symposium, St. Augustine, FL, USA; Feb 24-Mar 2, 2001 (canceled)

41. **"Insights on the dielectric breakdown in transistors from density functional calculations"** Conference on *"Applied Density Functional Theory"*, Vienna, Austria; Jan 14-17, 2001

42. **"Hydrogen electrochemistry in SiO_2 related to breakdown in gate oxides"** Third Japan-Korea Joint Workshop on *"First-Principles Electronic Structure Calculations"*; Tsukuba, Japan; Oct 30-Nov 1, 2000

43. **"Hydrogen electrochemistry in SiO_2 related to breakdown in gate oxides"** Psi-k 2000 Conference; Schwäbisch Gmünd,Germany; August 22-26, 2000

44. **"Hydrogen electrochemistry in SiO_2 related to breakdown in gate oxides"** March Meeting of the American Physical Society, Minneapolis, MN, USA; March 20-24, 2000

45. **"All-electron Car-Parrinello simulations of reactive processes in silicates"** Workshop on *"Fifteen years of the Car-Parrinello method in physics and chemistry"*, Minneapolis, MN, USA; March 18-19, 2000

46. **"Defect chemistry in silica related to dielectric breakdown in gate oxides"** 30th IEEE Semiconductor Interface Specialists Conference; Charleston, SC, USA; December 2-4, 1999

47. **"The role of hydrogen in silica"** Workshop on the *"Si-SiO_2 and SiC-SiO_2 interfaces – Similarities and Differences"*; Vanderbilt University, Nashville, TN; November 4-5, 1999

48. **"First-principles results on the defect chemistry in gate oxides"** Symposium on materials science at IBM; Yorktown Heights, NY, USA; November 1-2, 1999

49. **"Defect chemistry in silica"** Workshop on *"Frontiers in Fermion Quantum Monte Carlo Methods"*; Seattle, WA, USA; Sept. 22-26, 1999

50. **"Computational Physics and Chemistry"** Swiss-US-Forum on "Nanoscience and Nanotechnology"; Zurich, Switzerland; Sept. 20-22, 1999

51. **"Hydrogen Electrochemistry in Silica and the Origin of Stress-Induced Leakage Currents if MOSFEts"** 20th International Conference on "Defects in Semiconductors"; Berkeley, CA, USA; July. 26-30, 1999

52. **"Search for New Hydroamination Catalysts"** International workshop on "Probing Potential Energy Surfaces"; Zermatt, Switzerland; Apr. 17-23, 1999

53. **"The Projector Augmented Wave Method: Basics and Applications"** Spring Meeting of the American Chemical Society; Anaheim, CA, USA; Mar. 22-25, 1999

54. **"Ab-initio Molecular Dynamics of Water and Methanol in Zeolites"** 13th Canadian Symposium on Theoretical Chemistry; Vancouver, Canada; Aug. 2.-7, 1998

55. **"Ab-initio Molecular Dynamics Simulations in Search for New Hydroamination Catalysts"** Spring Meeting of the American Chemical Society; Dallas, TX, USA (presented by H.M. Senn); Mar. 27, 1998

56. **"Dynamics and Reactions of Molecules in Zeolite Catalysts"** CECAM Workshop on "Reactivity on Surfaces", Lyon, France; Aug. 28.-30, 1997

57. **"Dynamics and Reactions of Molecules in Zeolite Catalysts"** QTS'97: Symposium on Quantum Theory and Simulation of Bulk, Surface and Interface Phenomena; Raleigh, NC, USA; Jun. 15-18, 1997

58. **"The Projector Augmented Wave Method"** Psi-k Network Conference;
Schwäbisch Gmünd, Germany; Sept. 17-21, 1996

59. **"Atomistic Simulations"** Workshop on Nanoscience; Hasliberg, Switzerland; Oct. 14-18, 1996

60. **"Ab-initio Calculations on Enzyme and Zeolite Systems"** Workshop on Large Scale Electronic Structure Calculations; National Institute for Advanced Interdisciplinary Research, Tsukuba, Japan; Apr. 8, 1996

61. **"Enantioselective Catalysis with the Projector Augmented Wave Method"** Total Energy and Force Workshop; Paris, France; Jan. 9-12, 1996

62. **"Novel Approaches to solve Kohn-Sham Equations"** CECAM Specialist Workshop on "Density Functional Methods in Chemistry – Assessment and Opportunities"; Lyon, France; Jun. 28-30, 1995

63. **"Interaction of a Methanol with a Zeolite Acid Site"** International Symposium on Ab-Initio Molecular Dynamics; Zermatt, Switzerland; Apr. 22-29, 1995

64. **"The Projector Augmented Wave Method and Dynamical Properties of Organometallic Compounds"** International Symposium on Ab-Initio Molecular Dynamics; Zermatt, Switzerland; Apr. 22-29, 1995

65. **"The Projector Augmented Wave Method and Dynamical Properties of Organometallic Compounds"** Spring 1995 Meeting of the American Chemical Society; Anaheim, CA, USA; Apr. 2-7, 1995

66. **"Ab-Initio Molecular Dynamics of Organometallic Compounds"** 18th Gwatt Workshop: Computational Physics and Chemistry; Gwatt, Switzerland; Sept. 29-Oct. 1, 1994

67. **"Electronic Structure and Dynamical Properties of Organometallic Compounds"** Computational Material Science: Electronic Structure and Transport Properties; Nancy, France; Apr. 13-14, 1994

68. **"Electronic Structure of the Enzyme Superoxide Dismutase and the Binding of the Substrate"** Miniworkshop on Computational Condensed Matter Physics: Total Energy and Force Methods; Lyngby, Denmark; Jan. 6-9, 1994

69. **"PAW: An All-Electron Method for First-Principles Molecular Dynamics"** European Research Conference "Electronic Structure of Solids: Surfaces, Interfaces and Localized Defects"; Porto Carras, Greece; Sept. 18-23, 1993

70. **"PAW: An All-Electron Method for First-Principles Molecular Dynamics"** Workshop "The Electronic Structure of Condensed Matter"; Kreuth, Germany; Sept. 15-18, 1993

71. **"PAW: An All-Electron Method for First-Principles Molecular Dynamics"** CCP3-CCP9 Workshop "Electronic Structure Calculations using Non-Spherical 'Atomic' Potentials", Warrington, United Kingdom; Sept. 4-5, 1993

72. **"PAW: An All-Electron Method for First-Principles Molecular Dynamics"** Flamingo Workshop; Cagliari, Italy; Aug. 22-28, 1993

73. **"The Electronic Structure of the Cu,Zn Superoxide Dismutase Active Site and its Interaction with the Substrate"** Congres National de la Societe Francaise de Physique; Toulouse, France; Jul. 5-9, 1993

74. **"PAW: An All-Electron Method for First-Principles Molecular Dynamics"** 5th Annual Workshop for Electronic Structure Algorithms; State College, PA, USA; May 22-24, 1993

75. **"All-Electron Molecular Dynamics"** March meeting of the American Physical Society; Seattle, WA, USA; Mar. 22-26, 1993

76. **"Computational Methods"** "Swiss Initiative for Nanoscience and Technology"; Chaumont, Switzerland; Feb. 19-20, 1993

77. **"Self-Diffusion in Silicon"** Miniworkshop on "Methods of Electronic Structure Calculations", Trieste, Italy; Aug. 10-21, 1992

78. **"PAW: An All-Electron Method for First-Principles Molecular Dynamics"** Miniworkshop on "Methods of Electronic Structure Calculations"; Trieste, Italy; Aug. 10-21, 1992

79. **"First-Principles Calculations of Self-Diffusion Coefficients in Silicon"** Gordon Research Conference on "Point Defects, Line Defects and Interfaces in Semiconductors"; Plymouth, NH, USA; Jun. 20-24, 1992

80. **"First-Principles Calculations of Self-Diffusion Coefficients in Silicon"** Fifth International Workshop on Computational Condensed Matter Physics; Trieste, Italy; Jan. 16-18, 1991

81. **"Novel Hypothetical Carbon Modifications"** Miniworkshop on Fullerenes; IBM Zurich Research Laboratory, Switzerland; Sept. 2, 1992

82. **"Structure and Concentration of Self Interstitials in Silicon"** 20th International Conference on the Physics of Semiconductors; Thessaloniki, Greece; Aug. 6-10, 1990

83. **"First-Principles Calculations of Diffusion Coefficients: Hydrogen in Silicon"** Second Annual Workshop on Numerical Methods for Electronic Structure; Columbus, OH, USA; May 21-24, 1990

84. **"Dipols and Schottky-Barrier Heights of (111) $NiSi_2$/Si Interfaces"** 4th International Workshop on Computational Condensed Matter Physics "Total Energies and Force Methods", Trieste, Italy; Jan. 4-6, 1989

85. **"The Tight-Binding LMTO Method: From ASA to Full Potential"**
CECAM Workshop "Calculation of Electronic, Structural and Lattice Dynamical Properties of Semiconductor Interfaces and Surfaces" Orsay, France; Jun. 1989

86. **"Total Energies, Forces and Metal-Semiconductor Interface Calculations with the LMTO Method"** Miniworkshop on "Computational Condensed Matter Physics: Total Energy and Force Methods" Glion, Switzerland; Feb. 24-26, 1988

Invited Seminars

1. **"Exploring Materials Processes from first principles: Examples and Challenges"** Humboldt University, Berlin; Jan. 30, 2010

2. **"Auf dem Weg zum molekularen Design von Grenzflächen ab-Initio: Epitaktische Oxid-Halbleitergrenzflächen für kommende Transistorgenerationen (On the Road to a Molecular Design of Interface ab-Initio: Expitaxial Oxide-Semiconductor Interfaces for Future Transistor Generations)"** Kolloquium University of Erlangen, Germany; Jun. 9, 2008

3. **"Auf dem Weg zum molekularen Design von Grenzflaechen auf der Basis von Dichtefunktionalrechnungen"** Kolloquium of the Sonderforschungsbereich 602, Georg August University Göttingen, Germany; Apr. 25, 2008

4. **"Molekulares Design von Grenzflächen auf der Basis von Dichtefunktionalsimulationen (Molecular Design of Interfaces based on Density Functional Theory)"** H.C. Starck, Goslar, Germany; Dec. 1, 2006

5. **"The Projector-augmented wave method and the CP-PAW code: Basics and Applications"** BASF, Ludwigshafen, Germany; Nov. 24, 2006

6. **"How Nature breaks the strongest bond: Insights on the workings of Nitrogenase from first principles calculations."** Gemeinsames Seminar des Lehrstuhls für Theoretische Chemie und des Computer Chemie Centrum der Universität-Erlangen, Erlangen, Germany; Feb. 13, 2006

7. **"How does Nature Break the Strongest Bond: First principles Simulations of the Enzyme Nitrogenase"** Theoretisch-Chemisches Seminar der Ruhr-Universität Bochum; Bochum, Germany; Jul. 28, 2004

8. **"Interfacing Silicon with High-K Oxides"** Anorganisch Chemisches Kolloquium der Rheinland-Westfälischen Technischen Hochschule (RWTH); Aachen, Germany; Feb. 14, 2003

9. **"Insights on Gate Oxides in MOSFETs from First-Principles Simulations"** Dow Chemicals Central Research and Development, Midland, MI, USA; Jul. 29, 2002

10. **"Insights on Gate oxides in MOSFETs from first principles"** Condensed Matter Seminar, University of Basel, Switzerland; Feb. 4, 2002

11. **"Wave Function Thermostats in the Car-Parrinello Method"** Theory Seminar, Fritz Haber Institute of the MPG, Berlin, Germany; Nov. 1, 2001

12. **"Hydrogen Electrochemistry in Silica and Implications for MOSFETs"** Seminar Group Hofmann, University of Hannover, Hannover, Germany; Jul. 6, 2001

13. **"An Introduction to the Projector Augmented Wave Method"** Seminar, Frenking group Gerhard Mercator Universität, Marburg, Germany; Jun. 1, 2001

14. **"Hydrogen Electrochemistry in Silica and Implications for MOSFETs"** Materials Science Seminar, Princeton University, Princeton, NJ, USA; Dec. 6, 1999

15. **"Quantensimulationen in Physik und Chemie"** KFA Jülich, Germany; Nov. 19, 1999

16. **"Quantensimulationen in Physik und Chemie"** Heinrich Heine University Düsseldorf, Germany; Nov. 17, 1999

17. **"Hydrogen Electrochemistry in Silica and Implication on MOSFETs"** IBM Thomas J. Watson Research Center, Yorktown Heights, NY, USA; Sept. 30, 1999

18. **"Quantensimulationen in Chemie und Materialforschung"** Ludwig Maximilians University, Munich, Germany; Jul. 19, 1999

19. **"Quantensimulationen in Chemie und Materialforschung"** Clausthal University of Technology, Germany; May. 4, 1999

20. **"First-principles Calculations of Defects in Silica and the Origin of Stress-induced Leakage Currents in MOSFETs"** Solid State Physics Seminar; Vanderbilt University, Nashville, TE, USA; Feb. 5, 1999

21. **"First-principles Calculations of Defects in Silica and the Origin of Stress-induced Leakage Currents in MOSFETs"** IBM T.J. Watson Research Center, Yorktown Heights, NY, USA; Feb. 2, 1999

22. **"Tricks and Tips for the PAW Method"** Group Seminar, University of California – Los Angeles, USA; Jan. 28, 1999

23. **"Hydrogen Electrochemistry in Silica and Implication for MOSFETs"** Physical Chemistry Seminar, University of California – Los Angeles, USA; Jan. 27, 1999

24. **"The Projector Augmented Wave Method"** Group Seminar, University of California – Los Angeles, USA; Jan. 26, 1999

25. **"First Principles Calculations of Defects in Silica and the origin of Stress-induced leakage Currents in MOSFETs"** Computational Chemistry Seminar, Vienna University of Technology, Austria; Jan. 19, 1999

26. **"First Principles Calculations of Defects in Silica and the Origin of Stress-induced Leakage Currents in MOSFETs"** Institute Romand de la Recherche Materiaux, Lausanne, Switzerland; Dec. 12, 1998

27. **"Ab-initio Molecular Dynamics Simulations: In Search of new Hydroamination Catalysts"** Computational Chemistry Seminar; Vienna University of Technology, Austria; May 5, 1998

28. **"A New Wavefunction Thermostat"** Group Seminar; Vienna University of Technology, Austria; May 4, 1998

29. **"First-Principles Investigation of the Interaction of Water and Methanol with Acid Zeolites"** University of Calgary, Canada; Jun. 27, 1997

30. **"Principles of the Projector Augmented Wave Method"** Group Seminar, University of Calgary, Canada; June 25, 1997

31. **"First-Principles Calculations for Catalysis"** Max Planck Institut für Kohlenforschung, Mühlheim an der Ruhr, Germany; May 13, 1997

32. **"Barriers in the Nano-world"** Habilitationskolloquium Vienna University of Technology, Austria; May 7, 1997

33. **"Interaction of Methanol and Water with Zeolite Catalysts: An Ab-Initio Molecular Dynamics Study"** University of Zurich, Switzerland; Dec. 4, 1996

34. **"Density Functional Calculations for Enantio-Selective Catalysis: Allylic Amination with Fe,Pd Complexes Bearing P,N Ligands"** National Institute for Advanced Interdisciplinary Research, Tsukuba, Japan; Apr. 4, 1996

35. **"The Projector Augmented Wave method"** National Institute for Advanced Interdisciplinary Research, Tsukuba, Japan; Apr. 5, 1996

36. **"Molekulardynamik: Wechselwirkung von Wasser und Methanol in Zeolithen"** Seminar Computational Chemistry (158.003), Vienna University of Technology, Austria; Mar. 22, 1996

37. **"Enantioselektive Katalyse mittels Dichtefunktionalrechnungen: Asymmetrische Aminierung mit Pd Komplexen"** Seminar Computational Chemistry (158.003), Vienna University of Technology, Austria; Mar. 21, 1996

38. **"First-Principles Calculations for Catalysis"** Institute Romand de la Recherche Materiaux, Lausanne, Switzerland; Oct. 11, 1995

39. **"The Projector Augmented Wave Method and Dynamical Properties of Organometallic Compounds"** Seminar of the Sonderforschungsbereich 166 entitled "Strukturelle und magnetische Phasenübergänge in Übergangsmetall-Legierungen und –Verbindungen", Gerhard Mercator Universität, Duisburg, Germany; Jun. 21, 1995

40. **"The Projector Augmented Wave Method: An All-Electron Method for Electronic Structure Calculations"** Max-Planck work-group "Elektronensysteme", Dresden, Germany; Jun. 3, 1994

41. **"Self-Diffusion in Silicon"** Seminar, Vienna University of Technology, Vienna, Austria; 1992

42. **"Self-Diffusion in Silicon"** Theory Seminar, Fritz Haber Institut Berlin, Germany; Dec. 3, 1992

43. **"Electronic Structure Calculations at the Limiting Edge"** IBM Zurich Research Laboratory, Rüschlikon, Switzerland; Feb. 26, 1990

44. **"Self-Diffusion in Silicon"** Vienna University of Technology, Austria ; Nov. 16, 1992

45. **"Electronic Structure of Heterophase Boundaries – a Realistic Metal-Ceramic Interface"** Materials Science and Engineering Colloquium, Cornell University, Ithaka, NY, USA; May 3, 1990