

## Proposal for the Workshop

# Non-Adiabatic Dynamics at Surfaces

Schloss Reisenburg, 89321 Günzburg/Donau, Germany

22.-25. October 2007

### Abstract

Studying chemical reactions requires a detailed knowledge of the underlying potential-energy surfaces (PESs) that govern the nuclear motion. There is growing experimental evidence that many dynamic processes at surfaces are non-adiabatic, i.e., excited states of the system play an important role and the process can no longer be described by the Born-Oppenheimer ground state PES alone. The aim of the proposed workshop is to bring together scientists working on different approaches for excited state PESs to discuss and promote advances in this field. Applications to recent experimental results will be discussed with distinguished experimentalists.

### Scientific Summary

Assuming that electrons can react much faster to external perturbations than nuclei, the Born-Oppenheimer approximation is a widely employed approach to separate electronic and nuclear motion in dynamic processes. In this approximation the electrons adjust instantaneously to the slower movement of atoms, so that the atoms can be considered to move along a "potential energy surface" (PES) derived from a single electronic state. Focusing on motion on the electronic ground-state Born-Oppenheimer PES, modern many-body quantum-mechanical schemes like density-functional theory (DFT) have been highly successful in providing a parameter-free and often quantitative description of a variety of dynamical processes at solid surfaces. On the other hand, there is growing evidence that for many surface chemical reactions such an adiabatic approach fails to provide a sufficient description.

Electronically non-adiabatic gas-surface interactions have been discussed in order to account for dissociation dynamics observed in molecular beam experiments, or in the context of electron or light emission during adsorption at metal surfaces. Intimately connected to this are mechanisms of energy dissipation to the bulk solid, which, if hindered, could give rise to controversially debated processes like abstraction or "hot" adatom diffusion. A full quantum-mechanical treatment of these phenomena is severely challenged by the lowered symmetry at the solid surface, by the sheer size and complexity of the systems when considering the extended surface, as well as by the time scales over which it is necessary to follow the coupled atomic and electronic motion. Yet, in recent years this challenge has been increasingly taken up by algorithmic improvements and novel methodology. Insight into the diabatic or excited states energetics is increasingly provided by quantum chemistry, time-dependent or suitably

constrained DFT, as well as by the (self-consistent) GW approach, while the nuclear motion is propagated via wave packets or (quasi)classical dynamics. These developments have already significantly increased our atomic-scale understanding of non-adiabatic dynamics at solid surfaces. Still, substantial further advances are required in terms of basic theory. Furthermore, the strong methodological progress in each technique and in the various groups at different institutions is insufficiently coordinated at present. Strengths and weaknesses of the various approaches are therefore rarely critically compared, and interdisciplinary stimulations are low. The aim of the proposed workshop is to overcome this situation by bringing together leading experts, as well as Ph.D. students already working in the field and postdocs actively applying and developing the various theoretical techniques and simulation packages. Complemented by distinguished experimental colleagues, the focus will be on reviewing the current status and discussing the prospects and potential for further development and coupling of the various approaches. The intended format is that of a small dedicated workshop with about 50 participants. The meeting will be three days long and will take place in October 2007. In accordance with the character of the event as a workshop, sufficient time will be reserved for discussion, including a poster session for the graduate students and other emerging young scientists. The Wissenschaftszentrum Schloss Reisenburg close to Ulm (<http://www.uni-ulm.de/reisenburg/home.html>) offers a unique and ideal setting for the workshop and will stimulate information exchange and discussion in an informal atmosphere.

J. Behler, P. Rinke, K. Reuter, and M. Scheffler

## (Tentative) List of Invited Speakers and Discussion Leaders

Thorsten Klüner	U Oldenburg (D)	Quantum Chemistry
Oliver Kuehn	FU Berlin (D)	Quantum Chemistry
Nicola Marzari	MIT (USA)	Constrained-DFT
Troy van Voorhis	MIT (USA)	Constrained-DFT
Eckhard Pehlke	U Kiel (D)	TD-DFT
Hardy Groß	FU Berlin (D)	TD-DFT
Steven Louie	U Berkeley (USA)	GW, e-h Excitation
Angel Rubio	DIPC San Sebastian (E)	GW, e-h Excitation
Michael Rohlfing	U Osnabrück (D)	GW, e-h Excitation
Bengt Lundqvist	Chalmers (SE)	$\Delta$ SCF
Kiyoyuki Terakura	JRCAT-NAIR Tsukuba (J)	$\Delta$ SCF
Ronny Kosloff	Hebrew U Jerusalem (IL)	Quantum MD
Wolfgang Domcke	U München	Quantum MD
George Darling	U Liverpool (UK)	Wave Packet Dynamics
Stephen Holloway	U Liverpool (UK)	Wave Packet Dynamics
Dominik Marx	U Bochum	MD
Axel Gross	U Ulm (D)	MD, DFT
John Tully	Yale (USA)	Surface Hopping
Donald Truhlar	U Minnesota (USA)	Non-Adiabatic Dynamics
David Bird	U Bath (UK)	Non-Adiabatic Dynamics
Bill Gadzuk	NIST (USA)	e-h Excitation
Harald Brune	EPFL Lausanne (CH)	Hot Adatom Diffusion (exp.)
Bengt Kasemo	Chalmers (SE)	Electron Emission (exp.)
Eckart Hasselbrink	U Duisburg-Essen (D)	Molecular Beam Experiments
Bruce Kay	PNNL (USA)	Molecular Beam Experiments
Alec Wodtke	UCSB (USA)	Molecular Beam Experiments

## (Tentative) Budget

The workshop will start on October the 22<sup>nd</sup> in the afternoon and end at noon on October the 25<sup>th</sup> 2007. According to the price information provided by Schloss Reisenburg the cost for full board (breakfast, lunch, dinner, coffee breaks) and lodging during this time will amount to 300 Euro per participant. In addition, we intend to support the travel costs of the active participants. For this we adhere to the procedure employed to invited talks at the Dt. Physikalische Gesellschaft (DPG) spring meeting, i.e. reimbursement of the actual travel costs, up to a maximum of 100 Euro for participants from Germany and Switzerland, up to 400 Euro for participants from Europe, Scandinavia or the Middle East, up to 600 Euro for participants from East Coast USA, and up to 800 Euro for participants from West Coast USA or Asia.

Name:	Location:	Travel:	Local Costs:	Total:
David Bird	U Bath (UK)	400.-	300.-	700.-
Harald Brune	EPFL Lausanne (CH)	100.-	300.-	400.-
George Darling	U Liverpool (UK)	400.-	300.-	700.-
Wolfgang Domcke	TU München	100.-	300.-	400.-
Bill Gadzuk	NIST (USA)	800.-	300.-	1100.-
Axel Groß	U Ulm (D)	0.-	300.-	300.-
Hardy Groß	FU Berlin (D)	100.-	300.-	400.-
Eckart Hasselbrink	U Duisburg-Essen (D)	100.-	300.-	400.-
Stephen Holloway	U Liverpool (UK)	400.-	300.-	700.-
Bengt Kasemo	Chalmers (SE)	400.-	300.-	700.-
Bruce Kay	PNNL (USA)	600.-	300.-	900.-
Thorsten Klüner	U Oldenburg (D)	100.-	300.-	400.-
Oliver Kuehn	FU Berlin (D)	100.-	300.-	400.-
Ronny Kosloff	Hebrew U Jerusalem (IL)	400.-	300.-	700.-
Steven Louie	U Berkeley (USA)	800.-	300.-	1100.-
Bengt Lundqvist	Chalmers (SE)	400.-	300.-	700.-
Dominik Marx	U Bochum	100.-	300.-	400.-
Nicola Marzari	MIT (USA)	600.-	300.-	900.-
Eckhard Pehlke	U Kiel (D)	100.-	300.-	400.-
Michael Rohlfing	IU Bremen (D)	100.-	300.-	400.-
Angelo Rubio	DIPC San Sebastian (E)	400.-	300.-	700.-
Kiyoyuki Terakura	JRCAT-NAIR Tsukuba (J)	800.-	300.-	1100.-
Donald Truhlar	U Minnesota (USA)	600.-	300.-	900.-
John Tully	Yale (USA)	600.-	300.-	900.-
Troy van Voorhis	MIT (USA)	600.-	300.-	900.-

Alec Wodtke	UCSB (USA)	800.-	300.-	1100.-
	<b>Total:</b>	<b>9900.-</b>	<b>7800.-</b>	<b>17700.-</b>

We apply here for a partial support of 8000.- Euro to the total costs. As for the remaining costs, financial support will be applied at the Deutsche Forschungsgemeinschaft (DFG).

## Preliminary Workshop Program

### Monday, 22.10.2007

Noon – 16:00	Arrival and Registration
16:00 – 16:45	Talk 1
16:45 – 17:30	Talk 2
18:00 – 19:30	Dinner
19:30 – 20:15	Talk 3

### Tuesday, 23.10.2007

8:00 – 9:00	Breakfast
9:00 – 9:45	Talk 4
9:45 – 10:30	Talk 5
10:30 – 11:00	Coffee Break
11:00 – 11:45	Talk 6
11:45 – 12:30	Talk 7
12:30 – 14:00	Lunch
14:00 – 14:45	Talk 8
14:45 – 15:30	Talk 9
15:30 – 16:00	Coffee Break
16:00 – 16:45	Talk 10
16:45 – 17:30	Talk 11
18:00 – 19:30	Dinner
19:30 – ...	Poster Session

### Wednesday, 24.10.2007

8:00 – 9:00	Breakfast
9:00 – 9:45	Talk 12
9:45 – 10:30	Talk 13
10:30 – 11:00	Coffee Break
11:00 – 11:45	Talk 14
11:45 – 12:30	Talk 15
12:30 – 14:00	Lunch

14:00 – 14:45	Talk 16
14:45 – 15:30	Talk 17
16:00 – 19:00	Conference Outing
19:00 – 20:30	Dinner

**Thursday, 25.10.2007**

8:00 – 9:00	Breakfast
9:00 – 9:45	Talk 18
9:45 – 10:30	Talk 19
10:30 – 11:00	Coffee Break
11:00 – 11:45	Talk 20
11:45 – 12:30	Talk 21
12:30 – 14:00	Lunch and Departure

## Curriculum Vitae: Dr. Jörg Behler

### Dr. Jörg Behler

born 1975 in Hagen/Westf.

Postdoc

Eidgenössische Technische Hochschule, Zürich

Homepage: <http://www.rgp.ethz.ch/people/data/jbehler>



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### Scientific Curriculum

<b>1995 - 2000</b>	Chemie Diplom, Universität Dortmund
<b>2000 - 2004</b>	Dr. rer. nat., Fritz-Haber-Institut/Technische Universität Berlin
<b>2004 - 2005</b>	Postdoc, Fritz-Haber-Institut, Theory Dept. (Dr. K. Reuter, Prof. M. Scheffler)
<b>Since 2006</b>	Postdoc, ETH Zürich, Dept. of Chemistry and Applied Biosciences (Prof. M. Parrinello)

### Honors and Awards

Otto Hahn Medal of the Max-Planck Society 2005

Winner of the "Young Investigator Competition", Gordon Research Conference on Dynamics at Surfaces, Andover, NH, USA 2003

"Jahresbestenpreis" of the Chemistry Department, University of Dortmund, 2000

### Invited Speaker at International Conferences

Workshop: Bridging Time and Length Scales in Materials Science and Bio-Physics, UCLA, Los Angeles, USA 2005

Workshop: Probing Potential Energy Surfaces, Zermatt, Switzerland 2005

Conference: Catalysis from First Principles, Birkerød, Denmark, 2004

### Major Research Areas and Scientific Highlights

Non-adiabatic effects in gas-surface dynamics: Density-functional theory, ab initio molecular dynamics, representation of high-dimensional potential-energy surfaces with neural networks. Materials and systems: adsorption and dissociation of small molecules at metal surfaces, in particular oxygen at aluminium.

Phase transitions of crystalline solids under extreme conditions: Metadynamics. Materials and systems: Silicon, Carbon

### 5 Selected Publications of the last 5 years:

1. J. Behler, B. Delley, K. Reuter, and M. Scheffler: Diabatic potential-energy surfaces by constrained density-functional theory, submitted to *Phys. Rev. B*.
2. C. Ratsch, A. Fielicke, A. Kirilyuk, J. Behler, G. von Helden, G. Meijer, and M.

Scheffler: Structure determination of small vanadium clusters by density-functional theory in comparison with experimental far-infrared spectra, *J. Chem. Phys.* **2005**, 122, 124302.

3. A. Fielicke, A. Kirilyuk, C. Ratsch, J. Behler, M. Scheffler, G. Von Helden, and G. Meijer: Structure determination of isolated metal clusters via far-infrared spectroscopy, *Phys. Rev. Lett.* **2004**, 93, 023401.
4. J. Behler, B. Delley, S. Lorenz, K. Reuter, M. Scheffler: Dissociation of O<sub>2</sub> at Al(111): The role of spin selection rules, *Phys. Rev. Lett.* **2005**, 94, 036104.
5. R. Ludwig, J. Behler, B. Klink, and E. Weinhold: Molecular composition of liquid sulphur, *Angew. Chem. Int. Ed.* **2002**, 41, 3199.

## Curriculum Vitae: Dr. Patrick Rinke

### Dr. Patrick Rinke

born 1975 in Bad Oeynhausen  
Research Associate  
Fritz Haber Institute der Max Planck Society, Berlin  
Homepage: [www.fhi-berlin.mpg.de/th/member/rinke\\_p.html](http://www.fhi-berlin.mpg.de/th/member/rinke_p.html)



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### Scientific Curriculum

**1998 - 1999** Master of Science, University of York, England  
**1999 - 2002** Doctor of Philosophy (PhD), University of York, England  
**Since 2003** Research Associate, Fritz-Haber-Institut, Theory Dept. (Prof. M. Scheffler)

### Scholarships and Prizes

DAAD research scholarship (1998-1999, 2000-2001)  
EPSRC PhD studentship (1999-2002)  
Thesis Prize - Institute of Physics (UK) Computational Physics Group

### Cooperative Research Activities

EU Network of Excellence NANOQUANTA “*Nanoscale Quantum Simulations for Nanostructures and Advanced Materials*”

### Invited Speaker at International Conferences (selection out of 8 since 2004)

TDDFT Workshop: Prospects and Applications, Benasque, Spain 2006  
Psi<sub>k</sub> Conference, Schwäbisch-Gmünd, Germany 2005  
Nanoquanta Conference, Bad Honnef, Germany 2005, Maratea, Italy 2004  
Orbital Functionals for Exchange and Correlation, Berlin, Germany 2005

### Synergetic Activities (Conference Organization / Editorships)

Node leader and member of the Steering Committee of the EU Network of Excellence NANOQUANTA, organization of the NANOQUANTA Young Researcher Meeting 2005 and the NANOQUANTA annual workshop 2006

### Major Research Areas and Scientific Highlights

*Ab initio* theory of the electronic structure and quasiparticle excitations, in particular density-functional theory including novel, exact-exchange based functionals and self-energy methods (GW). Materials and systems: atoms, clusters, oxide films; semiconductor films, surfaces and bulk materials; II-VI compounds, nitrides, oxides, high-*k* materials

## 5 Selected Publications of the last five years:

1. P. Rinke, P., A. Qteish, M. Winkelkemper, D. Bimberg, J. Neugebauer, and M. Scheffler: Band gap and band parameters of InN and GaN from quasiparticle energy calculations based on exact-exchange density-functional theory. *Appl. Phys. Lett.* **2006** accepted
2. C. Freysoldt, P. Eggert, P. Rinke, A. Schindlmayr, R.W. Godby, and M. Scheffler: Dielectric anisotropy in the GW space-time method. *Comp. Phys. Comm.* **2006** accepted
3. P. Rinke, A. Qteish, J. Neugebauer, C. Freysoldt, M. Scheffler: Combining GW calculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. *New J. Phys.* **2005**, 7, 126.
4. K. Delaney, P. García-González, A. Rubio, P. Rinke, and R.W. Godby, Comment on "Band-gap problem in semiconductors revisited: Effects of core states and many-body self-consistency". *Phys. Rev. Lett.* **2004**, 93, 249701
5. P. Rinke, K. Delaney, P. García-González, and R.W. Godby, Image states in metal clusters. *Phys. Rev. A* **2004**, 70, 063201

## Curriculum Vitae: Dr. Karsten Reuter

### Priv.-Doz. Dr. Karsten Reuter

born 1970 in Offenbach/Main  
Head of Independent Junior Research Group  
Fritz Haber Institute der Max Planck Society, Berlin  
Homepage: [www.fhi-berlin.mpg.de/th/reuter/catalysis.html](http://www.fhi-berlin.mpg.de/th/reuter/catalysis.html)



### Scientific Curriculum

**1990 - 1995** Physik Diplom, Universität Erlangen-Nürnberg  
**1996 - 1998** Dr. rer. nat., Universität Erlangen-Nürnberg / Universidad Autónoma Madrid  
**1999 - 2002** Research Associate, Fritz-Haber-Institut, Theory Dept. (Prof. M. Scheffler)  
**2002 - 2003** DFG Scholarship Holder, FOM Instituut voor Atom en Molecuulfysica AMOLF, Amsterdam (Prof. D. Frenkel)  
**2003 - 2004** Group Leader "*Catalytic reactions at surfaces*", Fritz-Haber-Institut, Theory Department (Prof. M. Scheffler)  
**2005** Habilitation and venia docendi, FU Berlin, Physics Department  
**Since 2005** Head of MPG Independent Junior Research Group "*First-principles statistical mechanics*", Theory Department of the Fritz Haber Institute of the Max Planck Society

### Cooperative Research Activities

DFG Priority Program (Schwerpunktprogramm) SPP-1091 "*Bridging the gap between ideal and real systems in heterogeneous catalysis*", EU Specific Targeted Research Project (STREP) "*Oxidation of nanomaterials,  $\text{NiO}_2$* ", DFG Collaborative Research Centers (Sonderforschungsbereich) SFB-658 "*Molecular switches at surfaces*", EU Early Stage Training (EST) Network "*Molecular networks at phase boundaries*", EU COST Action P-19 "*Multiscale modeling of materials*", EPSRC Project "*Dynamic processes in the adsorption and formation of organic molecules on surfaces*"

### Invited Speaker at International Conferences (selection out of 68 since 2000)

KNAW Conference on Multiscale Modeling: Electrons, Molecules and Bio-Materials, Amsterdam 2006  
APS March Meeting, Baltimore 2006; Montreal 2004  
 $\text{Psi}_k$  Conference, Schwäbisch-Gmünd 2005  
Symposium on Surface Physics 2005 (SSP'05), Shizukuishi 2005  
5<sup>th</sup> Stranski-Kaischew Surface Science Workshop (SK-SSW'05), Pamporovo 2005  
10<sup>th</sup> Symposium on Surface Physics (SSP-10), Prague 2005  
American Conference on Theoretical Chemistry, Los Angeles 2005  
E-MRS Spring Meeting, Strasbourg 2004

## Synergetic Activities (Conference Organization / Editorships)

Member of the Int. Advisory Board for the “European Conference on Surface Crystallography and Dynamics” and the “International Workshop for Surface Physics”. Member of the Steering Committee of the EU COST Action P-19. Organization of 10 international workshops and conferences in the last 5 years.

## Major Research Areas and Scientific Highlights

Multi-scale modeling matching electronic structure theories with concepts from statistical mechanics and thermodynamics: Density-functional theory, atomistic (surface) thermodynamics, (kinetic) Monte Carlo simulations, *ab initio* molecular dynamics, *ab initio* lattice gas Hamiltonians (surface phase diagrams, TPD). Scattering theory and interaction of electrons and photons with solid surfaces (LEED, XPS, STM, HREELS). Materials and systems: metals, transition metals and oxides; adsorption and catalytic reactions at solid surfaces.

## 10 Selected Publications of the last 5 years from a total of 50 Refereed Publications

1. J. Schnadt, A. Michaelides, J. Knudsen, R. T. Vang, K. Reuter, E. Laegsgaard, M. Scheffler, F. Besenbacher: Revisiting the structure of the p(4x4) surface oxide on Ag(111), *Phys. Rev. Lett.* **2006**, 96, 146101.
2. K. Reuter, M. Scheffler: First-principles kinetic Monte Carlo simulations for heterogeneous catalysis: Application to the CO oxidation at RuO<sub>2</sub>(110), *Phys. Rev. B* **2006**, 73, 045433.
3. K. Reuter, C. Stampfl, M. Scheffler: *Ab initio* atomistic thermodynamics and statistical mechanics of surface properties and functions. In: *Handbook of Materials Modeling, Vol. 1*. (Ed.) S. Yip, Springer Berlin Heidelberg **2005**, 149-194. ISBN 1-4020-3287-0.
4. J. Behler, B. Delley, S. Lorenz, K. Reuter, M. Scheffler: Dissociation of O<sub>2</sub> at Al(111): The role of spin selection rules, *Phys. Rev. Lett.* **2005**, 94, 036104.
5. K. Reuter, D. Frenkel, M. Scheffler: The steady-state of heterogeneous catalysis, studied by first-principles statistical mechanics, *Phys. Rev. Lett.* **2004**, 93, 116105.
6. E. Lundgren, J. Gustafson, A. Mikkelsen, J. N. Andersen, A. Stierle, H. Dosch, M. Todorova, J. Rogal, K. Reuter, M. Scheffler: Kinetic hindrance during the initial oxidation of Pd(100) at ambient pressures, *Phys. Rev. Lett.* **2004**, 92, 046101.
7. K. Reuter, M. Scheffler: First-principles atomistic thermodynamics for oxidation catalysis: Surface phase diagrams and catalytically interesting regions. *Phys. Rev. Lett.* **2003**, 90, 046103.
8. J. Wang, C. Y. Fan, Q. Sun, K. Reuter, K. Jacobi, M. Scheffler, und G. Ertl: Surface coordination chemistry: Dihydrogen versus hydride complexes on RuO<sub>2</sub>(110), *Angew. Chemie Int. Edition* **2003**, 42, 2151.
9. K. Reuter, C. Stampfl, M. V. Ganduglia-Pirovano, M. Scheffler: Atomistic description of oxide formation on metal surfaces: The example of Ru, *Chem. Phys. Lett.* **2002**, 352, 311.
10. K. Reuter, M. Scheffler: Composition, Structure and Stability of RuO<sub>2</sub>(110) as a function of oxygen pressure, *Phys. Rev. B* **2002**, 65, 035406.

## Curriculum Vitae: Prof. Matthias Scheffler

### Prof. Dr. Matthias Scheffler

born 1951 in Berlin  
Director at the Fritz Haber Institute  
of the Max Planck Society, Berlin, Germany  
Homepage: [www.fhi-berlin.mpg.de/th/th.html](http://www.fhi-berlin.mpg.de/th/th.html)



### Scientific Curriculum

- 1978** Dr. rer. nat., Technical University Berlin, Physics Department  
**1978-1988** Scientific staff member of the Physikalisch-Technische Bundesanstalt, Braunschweig, Germany  
**1979-1980** Postdoc at the IBM T.J. Watson Research Center, Yorktown Heights, USA  
**1984** Habilitation and venia legendi, Technical University Berlin  
**Since 2001** Honorary Professor for Theoretical Physics, FU Berlin  
**Since 1989** Honorary Professor for Theoretical Physics, TU Berlin  
**Since 1988** Director at the Fritz Haber Institute of the Max Planck Society, Berlin  
**Since 2005** Distinguished Visiting Professor at the University of California, Santa Barbara

### Honors and Awards (selection)

- Since 1998 Fellow of the American Physical Society.  
2001 Max Planck Research Award for International Cooperation (AvH and MPG).  
Since 2002 Ordinary Member of the Berlin-Brandenburgischen Akademie der Wissenschaften.  
2003 Medard W. Welch Medal and Prize (AVS Science and Technology Society, USA).  
2004 Max Born Medal and Prize, (Institute of Physics, UK and DPG, Germany).

### Cooperative Research Activities

DFG Priority Program SPP 1091 *"Bridging the gap in heterogeneous catalysis"* (project leader), Partnership for International Research and Education at the University of California *"Electron Chemistry and Catalysis at Interfaces"* (principle investigator), EU Network of Excellence IDECAT *"Integrated Design of Catalytic Nanomaterials for a Sustainable Production"* (project leader), MPG-CAS Partner Group in Dalian, China *"First-Principles Theory of High-Pressure Oxidation Catalysis"* (governing board), EU Specific Targeted Research Project NanO<sub>2</sub> *"Oxidation of Nanomaterials"* (project leader), EU Early Stage Research Training MONET *"Molecular Networks at Phase Boundaries"* (governing board), EU Network of Excellence NANOQUANTA *"Nanoscale Quantum Simulations for Nanostructures and Advanced Materials"* (project leader, governing board), Australian Research Council Discovery Project *"Ab initio Theory in Complex Materials and Surfaces: Prediction and Design of Functional Structures"* (principle investigator), EU Network of Excellence SANDiE *"Self-Assembled Semiconductor*

*Nanostructures for New Devices in Photonics and Electronics*" (project leader, governing board) UCSB-MPG Program for International Exchange in Material Sciences (program coordinator), Institut Francaise du Pétrole PhD student program (supervisor), ESF Research Networking Program "Towards Atomistic Materials Design,  $\Psi_k$ " (governing board), ESF Marie Curie Human Resources and Mobility Action "Training in Computational Nanoscience,  $\Psi_k$ " (steering committee), ESF Research Networking Program SimBioMa "Molecular Simulations in Biosystems and Material Science" (case study coordinator).

### **Invited Speaker at International Conferences (100 in the last 5 years); selection:**

Inaugural Meeting "Center for Nanophase Materials Sciences" Oak Ridge, USA, 2005  
Int. Symposium on Surface Science and Nanotechnology (ISSS-4), Saitama, Japan 2005  
PacifiChem 2005 Conference, Honolulu, Hawaii, USA, 2005  
Advanced Workshop on Recent Developments in Inorganic Materials, Trieste, Italy, 2006  
Materials Research Outreach Symposium, University, Univ. California Santa Barbara, USA, 2006  
Winter School "Computational Nanoscience: Do it yourself", FZ Jülich, 2006

### **Synergetic Activities (Conference Organization / Editorships)**

Organizer and co-organizer of numerous conferences and workshops, member of various editorial boards, active in the DPG and APS on various levels

### **Major Research Areas and Scientific Highlights**

*Ab initio* theory of the electronic structure, in particular density-functional theory, quantum Monte Carlo, and self-energy methods (GW). *Ab initio* atomistic thermodynamics and *ab initio* statistical mechanics, in particular molecular dynamics and kinetic Monte Carlo methods, as well as lattice-gas Hamiltonians. Various hybrid methods that enable us to study mesoscopic systems and time spans from pico seconds to seconds. Materials studied include semiconductors, metals, transition-metal oxides, carbon nano structures, transition-metal clusters, and biomolecules. The main research goal is the understanding of the properties, metastabilities, dynamics and function of nanostructures (electronic, magnetic, structural, and chemical).

### **10 selected publications from 101 refereed papers since 2001:**

1. B. Li, A. Michaelides, M. Scheffler: "Textbook" adsorption at "nontextbook" adsorption sites: Halogen atoms on alkali halide surfaces. *Phys. Rev. Lett.* **2006**, 97, 046802.
2. P. Rinke, A. Qteish, J. Neugebauer, C. Freysoldt, M. Scheffler: Combining GW calculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors (35 pages). *New J. Phys.* **2005**, 7, 126.
3. J. Behler, B. Delley, S. Lorenz, K. Reuter, M. Scheffler: Dissociation of O<sub>2</sub> at Al(111): The role of spin selection rules. *Phys. Rev. Lett.* **2005**, 94, 036104.

4. K. Reuter, D. Frenkel, M. Scheffler: The steady state of heterogeneous catalysis, studied by first-principles statistical mechanics. *Phys. Rev. Lett.* **2004**, 93, 116105.
5. J. Ireta, J. Neugebauer, M. Scheffler: On the accuracy of DFT for describing hydrogen bonds: Dependence on the bond directionality. *J. Chem. Phys. A* **2004**, 108, 5692.
6. A. Fielicke, A. Kirilyuk, C. Ratsch, J. Behler, M. Scheffler, G. von Helden, G. Meijer: Structure determination of isolated metal clusters via far-infrared spectroscopy. *Phys. Rev. Lett.* **2004**, 93, 023401.
7. R. Pentcheva, K. A. Fichthorn, M. Scheffler, T. Bernhard, R. Pfandzelter, H. Winter: Non-Arrhenius behavior of the island density in metal heteroepitaxy: Co on Cu(001). *Phys. Rev. Lett.* **2003**, 90, 076101.
8. J. Ireta, J. Neugebauer, M. Scheffler, A. Rojo, M. Galván: Density functional theory study of the cooperativity of hydrogen bonds in finite and infinite  $\alpha$ -helices. *J. Phys. Chem. B* **2003**, 107, 1432; *J. Phys. Chem. B* **2003**, 107, 9616.
9. G.-J. Kroes, A. Gross, E.-J. Baerends, M. Scheffler, D. A. McCormack: Quantum theory of dissociative chemisorption on metal surfaces. *Acc. Chem. Res.* **2002**, 35, 193.
10. C. Filippi, S. B. Healy, P. Kratzer, E. Pehlke, M. Scheffler: Quantum Monte Carlo calculations of H<sub>2</sub> dissociation on Si(001). *Phys. Rev. Lett.* **2002**, 89, 166102.