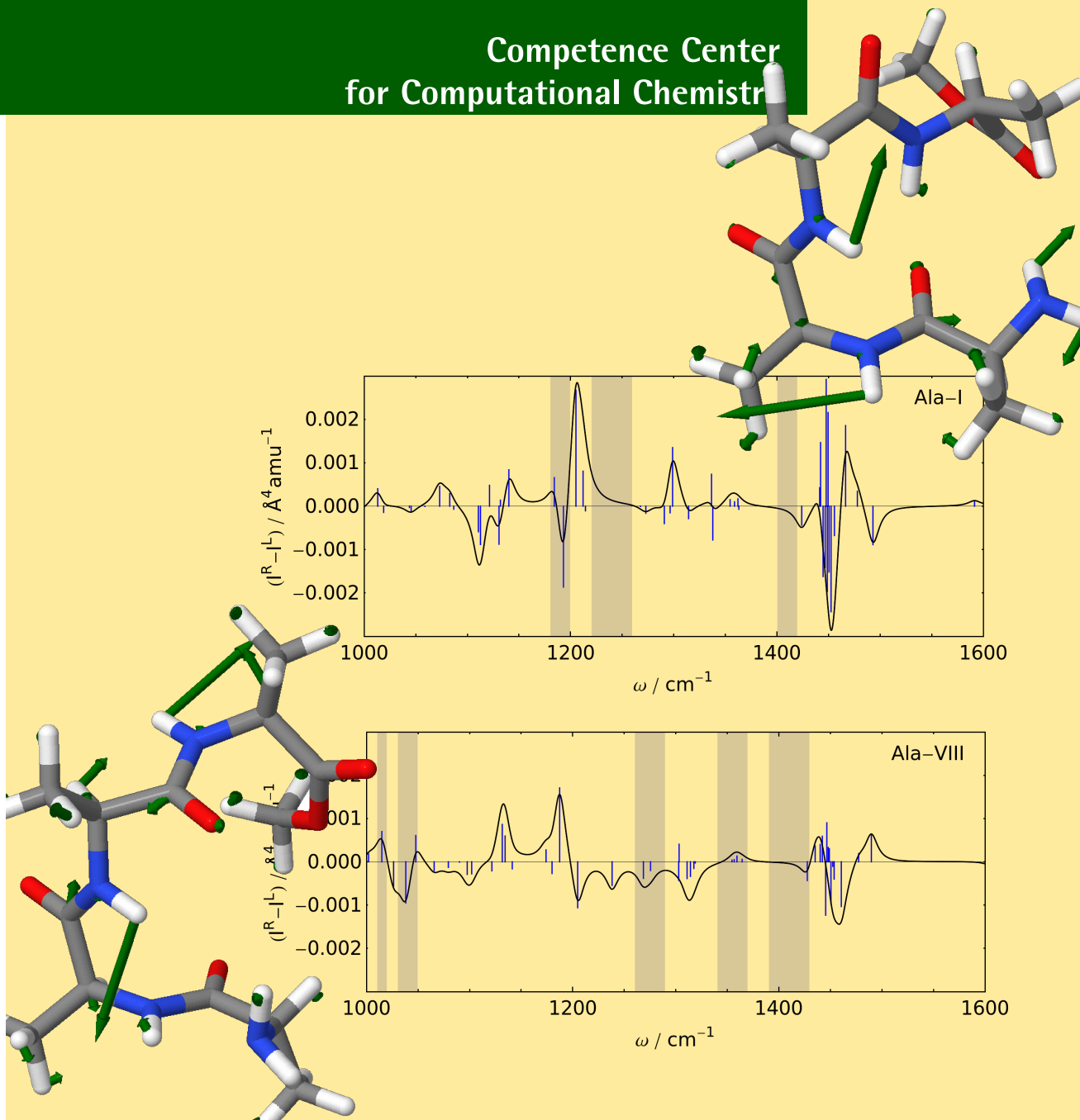
Annual Report 2011 / 2012

[C⁴]

Competence Center for Computational Chemistr



University of Zurich[UZH]

ETH Eidgenössische Technische Hochschule Zürich

Annual Report

[C4]

Competence Center for Computational Chemistry

July 2011 to June 2012

Impressum

Edited by:
Halua Pinto de Magalhães, ETH Zürich

Copies of this report are available from:
Christine Siegrist Pfister
Laboratorium für Physikalische Chemie
ETH Hönggerberg
CH-8093 Zürich
Tel. +41 44 632 7901
Fax +41 44 632 1021
Email: christine.siegrist@phys.chem.ethz.ch

C^4 on the Internet:
www.c4.ethz.ch

Cover:
Thomas Weymuth, one of the two winners of the 2011 IBM Research Forschungspreis

Quantum-chemical calculations allow for the identification of vibrational Raman optical activity signatures of different types of β-turns.

Printing:
Fröhlich Druck AG
www.froehlich.ch

Contents

1 About C^4

The Competence Center for Computational Chemistry [C^4] is a network of computational chemists of the IBM Zürich Research Laboratory, the University of Zürich, and the ETH Zürich. The goal of C^4 is to seek new frontiers and opportunities in molecular modeling and simulation, to cater to the flow of know-how within this community, and to serve as a platform for the interaction with partners from other areas of science or from outside academia. C^4 was launched twenty years ago as a scientific collaboration between the IBM Research Laboratory and ETH Zürich, and has grown considerably since. Today, the C^4 network covers a much broader spectrum of research activities, and its output in terms of scientific results and achievements is still on the increase.

The Steering Committee consists of Prof. Alessandro Curioni, head of computational sciences at IBM Zürich Research, Profs. Jürg Hutter (University of Zürich), Wilfred F. van Gunsteren, and PD Dr. Hans P. Lüthi (both ETH Zürich). C^4 does not know formal membership. A "member" defines itself by the involvement in the activities of C^4.

This is the 19th Annual Report of the Competence Center for Computational Chemistry [C^4] reporting on its activities between July 2011 and June 2012. We also encourage you to visit our website, www.c4.ethz.ch .

2 The Year in Review

About this C4 Annual Report

Over the past two decades, the C4 Network has grown substantially, and it became increasingly difficult to present the full scope of the research activities the Annual report. Therefore, last year, we decided to go for a change of format: the descriptions of individual projects were removed, and replaced by a page where each research group lists its research interests and, at the same time, directs the interested reader to its home page. This change of format turned out to make sense, and this way the Annual Report still gives a comprehensive overview over the activities of the computational chemistry community of the three partner institutions.

C4 Seminar

The actual "backbone" of C4 is its Seminar Program. During the 2011 Fall- and 2012 Spring-Term the C4 Seminar Program covered 14 lectures, again some of them presented by leaders in the field of computational chemistry. Two additional C4 seminars were hosted by the IBM Research Laboratory.

The seminar, which takes place every second Thursday during the semester, enjoys a remarkable popularity bringing together between forty and sixty students and researchers each time. The complete seminar program is listed in this report.

Compute Resource

In May 2011, after five years of uninterrupted service, the C4 compute-cluster Obélix, a 32 node quad-core IBM Opteron cluster operated by the Server Group of the ETH Informatikdienste, was decommissioned. At the same time the existing C4 Brutus share was extended by 10 standard and 5 fat nodes, i.e. a total of 720 cores, based on an infrastructure-grant of ETH and a matching financial contribution of the ETH Department of Chemistry and Applied Biosciences.

Many of the members of the C4 community have their own computing facilities, or have access to the central compute clusters. In addition, some members are users of the resources of the Centro Svizzero die Calcolo Scientifico (CSCS), i.e. were awarded computing time based on proposals they had submitted. Each of these resources respond to a specific demand, and the results and achievements reported in this report typically involve "machine cycles" drawn from more than just one of these resources.

C4 Tutorials

With CECAM being established in Switzerland, the offering for tutorials and workshops has increased considerably, both, in number and in the spectrum of topics covered. The CECAM Zurich node is lead by our colleague Prof. Matthias Troyer of the Institute of Theoretical Physics. C^4 did not offer its own tutorials.

The IBM Research Award

In 2007, the ETH Schulleitung approved the "IBM Research Forschungspreis", an award for outstanding MSc and PhD theses sponsored by the IBM Zürich Research Laboratory. This year, the prize was awarded to Marco Schweizer (D-MATL; Group of Prof. Ch. Oettinger) and Thomas Weymuth (D-CHAB; Group of Prof. M. Reiher) for their MSc theses entitled "simulation of dissipative quantum systems " and "Identifying Protein beta-Turns with Vibrational Raman Optical Activity", respectively.

The 2011 Award Ceremony, for the second time, took place at the ETH Tag, with the Rector, Prof. Heidi Wunderli-Allenspach, handing out the award to the winner. The two laureates also presented their research at the occasion of a special C^4 Seminar held on May 31, 2012, at the IBM Research Laboratory in Rüschlikon. For more detail please refer to the respective section in this report.

IBM Shared University Research (SUR) Grant Awarded to C4

Based on their grant proposal, Alessandro Curioni and Hans P. Lüthi were awarded an IBM Power 755 server with 32 POWER7 cores and 256 GBytes of (shared) memory. The server is dedicated to method development projects within the C^4 community.

Outlook

We hope that you will enjoy browsing through the "yellow pages" of "computational chemistry made in Zürich".

The C^4 Steering Committee would like to thank the community for its active participation in its program and activities. Also in the next year we will make sure that C^4 remains a valuable platform for the Zürich computational chemistry community.

Hans P. Lüthi, Leiter C^4
October 22, 2012

3 The C^4 Network & Areas of Research

The C^4 Network involves researchers from different participating institutions. The ETH Zürich is represented by the Departments of Chemistry and Applied Biosciences, Physics and Materials Science. Further, there are the Institute of Physical Chemistry and the Institute of Organic Chemistry at the University of Zürich as well as the IBM Zürich Research Laboratory.

Note that only a relatively small fraction of the research reported in this document was performed using C^4 compute resources; its capacity would be much to small to generate the scientific output listed here. The main idea behind this document is to have a compilation of the research in computational chemistry "made in Zürich", and to offer a listing of competencies and skills available.

The C^4 community

Research Group	*Institute*
Prof. K. Baldridge	Organic Chemistry UNI ZH
Prof. P. Chen*	Organic Chemistry ETH
Prof. C. Copéret	Inorganic Chemistry ETH
Prof. A. Curioni	IBM Zürich Research Laboratory
Prof. W. F. van Gunsteren	Physical Chemistry ETH
Prof. A. Gusev*	Polymers ETH
Prof. I. Hermans	Chemical and Bioengineering
Prof. P. Hünenberger	Physical Chemistry ETH

Research Group	*Institute*
Prof. J. Hutter	Physical Chemistry UNI ZH
PD Dr. H.P. Lüthi	Physical Chemistry ETH
Prof. R. Nesper	Inorganic Chemistry ETH
Prof. M. Parrinello	Physical Chemistry ETH
Prof. M. Quack	Physical Chemistry ETH
Prof. M. Reiher	Physical Chemistry ETH
Prof. G. Schneider*	Pharmaceutical Sciences ETH
Prof. F. Schoenebeck	Organic Chemistry ETH
Prof. N. Spaldin*	Materials Theory ETH
Prof. M. Troyer	Theoretical Physics ETH
Prof. V. Vogel*	Biologically Oriented Materials ETH
Prof. J. VandeVondele**	Biologically Oriented Materials ETH
Prof. P. Werner	Theoretical Physics ETH

*) No contributions for this year's report
**) Newly appointed

4 C4 Activities in 2011/2012

C4 Seminar

During the 2011 Fall- and 2012 Spring-Term the C4 Seminar Program covered 14 lectures, again some of them presented by leaders in the field of computational chemistry. Two additional C4 seminars were hosted by the IBM Research Laboratory.

C4 Tutorials

During the past year, there were no tutorials offered by C4 .

C4 Workshop

During the past year, there was no workshop offered by C4. Information about previous workshops can be found at www.c4.ethz.ch/seminarseries/index

On the next two pages you will find the C4 Seminar Programs.

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

COMPETENCE CENTER FOR COMPUTATIONAL CHEMISTRY C4
ETH Zürich / University of Zürich / IBM Research

Seminar Programm Herbstsemester 2011

Auditorium HCI J6 / J3, ETH Hönggerberg
13:00-14:00

29. 09. 2011
Prof. Carlos Aleman, Universitat Politècnica de Catalunya, Barcelona (Spain)
Molecular Dynamics Simulations on Large Systems:
From Peptide Nanowires to Dendronized Polymers

13. 10. 2011
Prof. Willem M. Klopper, Karlsruher Institut für Technologie (KIT),
Karlsruhe (Deutschland)
Coupled-Cluster Theory at the Basis-set Limit

27. 10. 2011
Prof. Alexander MacKerell, University of Maryland, Baltimore (MD, USA)
Progress Towards a Comprehensive Polarizable Macromolecular Force Field Based on the CHARMM Classical Drude Oscillator Model

10.11. 2011
Prof. Leeor Kronik, Weizmann Institute of Science, Rehovoth (Israel)
Spectroscopy With Density Functional Theory: New Ideas for an Old Problem

24. 11. 2011
Prof. Nicola Spaldin, ETH Zürich, Zürich (Schweiz)
Computational Materials and Cosmic Strings

01.12. 2011
Dr. Richard W. Pastor, National Institutes of Health (NIH), Bethesda (MD, USA)
Molecular Dynamics Simulations of Membrane Curvature

08. 12. 2011
Dr. Marcello Sega, Universität Stuttgart, Stuttgart (Deutschland)
Computing Dielectric Properties of Charged Soft-Matter

www.c4.ethz.ch

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

COMPETENCE CENTER FOR COMPUTATIONAL CHEMISTRY C4
ETH Zürich / University of Zürich / IBM Research

Seminar Programm Frühjahrssemester 2012

Auditorium HCI J7, ETH Hönggerberg
13:00-14:00

01. 03. 2012
Prof. Núria López, Institut Català d'Investigació Química, Tarragona (Spain)
Selectivity in Hydrogenation Reactions: the Role of Theoretical Simulations

15. 03. 2012
Prof. Dr. Patrick Bultinck, Ghent University**,** Ghent (Belgium)
The Fukui matrix, an algebraic tool for the understanding of Fukui functions, their magnitude and sign and effects of correlation and degeneracy

12. 04. 2012 **Easter Break** (no seminar)

26. 04. 2012
Dr. Hans Martin Senn, Lecturer, University of Glasgow, Glasgow, Scotland (UK)
Insights into enzymatic catalysis using computational chemistry:
From docking to coupled-cluster methods.

03. 05. 2012
Prof. Alán Aspuru-Guzik, Harvard University, Cambridge, MA (USA)
Finding renewable energy materials using one screensaver at a time:
The Harvard Clean Energy Project

10. 05. 2012
Dr. Saron Catak, Center for Molecular Modeling, Ghent University, Zwijnaarde, (Belgium)
First principles metadynamics simulations of 'Rare Events' in biological systems

24. 05. 2012
Prof. Tim Clark, Friedrich-Alexander-Universität Erlangen-Nürnberg,
Erlangen (Germany)
Simulating soft electronic devices:
High-performance NDDO calculations for new materials

www.c4.ethz.ch

5 IBM Research Forschungspreis

2007 Sandra Luber (Group of Prof. M. Reiher)
Towards the Calculation of Raman Optical Activity Spectra of Large Molecules

2008 Daan Geerke (Group of Prof. W.F. van Gunsteren)
Classical Hamiltonians in Molecular Simulation: Force-Field Development and Explicit Inclusion of Electronic Polarization and Quantum Effects

2009 Sereina Riniker (Group of Prof. W.F. van Gunsteren)
Free Energies of Binding of Benzene Derivatives to Alpha-Cyclodextrin: Sensitivity of the Free-Energy Components to Temperature and to the Restraining of Molecular Motion

2010, Michele Ceriotti (Group of Prof. M. Parrinello)
"A novel framework for enhanced molecular dynamics based on the generalized Langevin equation"

In support of computer modeling and simulation, the IBM Research Zurich Laboratory donated a prize for outstanding Masters and PhD theses in the areas of computational chemistry, physics, biology, and materials science in 2007. In even-numbered years, the Call for Nominations is for PhD theses, in odd-numbered years it is for MS theses.

The Call for Nominations for the 2012 IBM Research Forschungspreis was issued at the end of the Spring Term. It is for PhD theses submitted during the past two years.

The Winners of the 2011 IBM Research Prize

The Award Jury, consisting of Profs. Alessandro Curioni, U.W. Suter and PD Dr. H.P. Lüthi awarded Marco Schweizer and Thomas Weymuth the IBM Research Forschungspreis for their innovative MSc theses.

Marco Schweizer (H.C. Oettinger group)
"Simulation of Dissipative Quantum Systems"

Thomas Weymuth (M. Reiher group)
"Can Raman Optical Activity Discriminate Between Different Types of Protein Beta-Turns?"

Marco Schweizer and Thomas Weymuth with the Rektorin, Prof. Heidi Wunderli-Allenspach, and Prof. Alessandro Curioni at the ETH-Tag 2011

Marco Schweizer

Departement of Materials ETH Zürich

MSc Thesis 2010

"Simulation of Dissipative Quantum Systems"

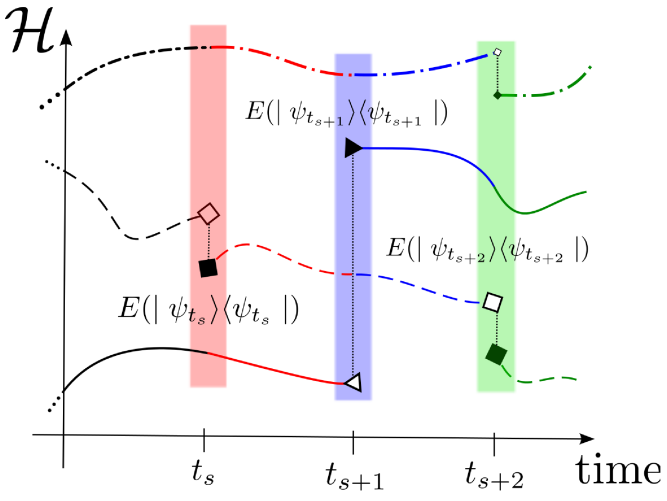


Illustration of the Monte-Carlo technique:
stochastic evolution of trajectories in the quantum system of interest.

In all relevant real world applications quantum systems are exposed to their environment possessing an overwhelming number of degrees of freedom so that the exact evolution of the composite system becomes impossible to solve numerically. A coarse-grained approach in the spirit of thermodynamics that focuses only on the relevant features of the system was developped [1]; the environment is treated thermodynamically and most strikingly dynamically while being coupled to the quantum system of interest. The latter is described by a highly nonlinear quantum master equation with many appealing thermodynamic properties as opposed to linear frameworks. In the thesis it is shown that despite of the nonlinear structure problems can be solved by a Monte-Carlo technique. In addition, common stochastic integration schemes are extended and improved to obtain higher order of convergence. While results are presented to the prototypical toy model of a simple qubit coupled to a classical heat bath, extensions are highlighted to treat much more involved problems.

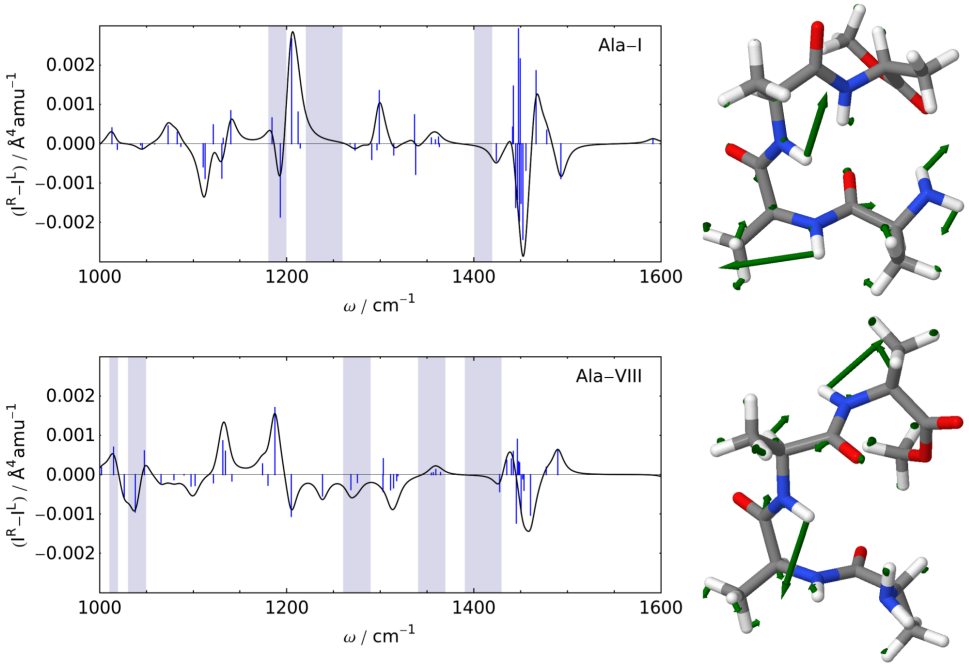
[1] H. C. Öttinger, *Phys. Rev. A* 82, 052119 (**2010**)

Thomas Weymuth

Laboratory of Physical Chemistry ETH Zürich

MSc Thesis 2010

"Can Raman Optical Activity Discriminate Between Different Types of Protein Beta-Turns?"



β-turns belong to the most important secondary structure elements in proteins. On the basis of density functional calculations, vibrational Raman optical activity signatures of different types of β-turns were established and compared as well as related to other signatures proposed in the literature earlier. Our findings indicated that there are much more characteristic ROA signals of β-turns than have been hitherto suggested. These suggested signatures were, however, found to be valid for the most important type of β-turns. Moreover, we compared the influence of different amino acid side chains on these signatures and investigated the discrimination of β-turns from other secondary structure elements, namely α- and 3_{10}-helices.

6 The C4 Compute Resources

IBM Cluster e1350 "Obélix"

Obélix, a 32 node IBM cluster was decommissioned on the July 30, 2011, after an uninterrupted uptime of 1'846 days of the fileserver, the most essential part of the cluster. The Obélix cluster served more than 100 users over more than 6 years as a reliable computing facility. By this date, an era reached its end: Obélix was the last stand-alone compute server for C4.

Brutus Share

As a replacement, C4 obtained and extension of its existing Brutus share. Based on an infrastructure proposal supported by the Department of Chemistry and Applied Biosciences (D-CAB), the VP Research granted an extension of the active share on Brutus by another ten standard- and five fat-nodes. The fifteen nodes with 48 cores each (12 core AMD 6174 CPUs; 4CPUs per node). The 720 core share went into production in November 2011. At this point, the D-CHAB is the biggest Brutus shareholder.

7 Research Group Portraits & Publications in 2011/2012

Overview

Group of Kim K. Baldridge
Organic Chemistry Institute
UZH Zürich

www.oci.uzh.ch/research/baldridge.html

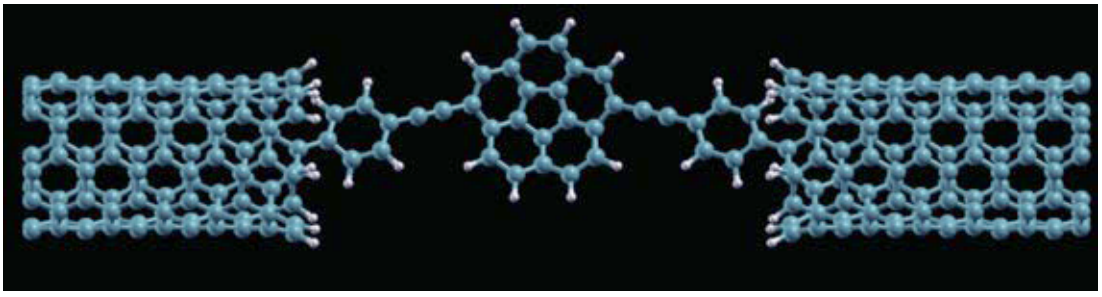
Areas of Research:

Electronic Structure Theory Development and Applications, Computational Science, Grid Technologies

Keywords:

Quantum Chemistry, Electronic Transport, Optical Properties, Chemical reactivity, Dispersion-DFT

Main research topics:



References

Zoppi, L.; Martin-Samos, L.; Baldridge, K.K.
Effect of molecular packing on corannulene-based materials electroluminescence.
J. Am. Chem. Soc., 133, 14002 (**2011**).

Bauert, T.; Baldridge, K.K.; Siegel, J.S.; Ernst, K.-H
Surface-assisted bowl-in-bowl stacking of nonplanar aromatic hydrocarbons,
ChemComm, 47, 7995 (**2011**).

Romanato, P.; Duttwyler, S.; Linden, A.; Baldridge, K.K.; Siegel, J.S.
Competition between π-Arene and Lone Pair-Halogen Stabilization in Silylium Ions.
J. Am. Chem. Soc., 133, 11844 (**2011**).

Bauert, T.; Zoppi, L.; Koller, G.; Garcia, A.; Baldridge, K.K.; Ernst, K.-H.
Large Induced interface Dipole Moments without Charge Transfer: Buckybowls on Metal Surfaces.
J. Phys. Chem. Lett., 2 (21), 2805 (**2011**).

Frantz, D.K.; Linden, A.; Baldridge, K.K.; Siegel, J.S.
Molecular Spur Gears Comprising Tryptycene Rotators and Bibenzimidazole-Based Stators.
J. Am. Chem. Soc., 134, 1528 (**2012**).

Car, P.-E.; Guttentag, M.; Baldridge, K.K.; Alberto, R.; Patzke, G.
Polyoxometalate water oxidation catalysts: a new open triruthenium silicotungstate vs. Co- and Ni-sandwich analogues.
Green Chem., 14, 1680 (**2012**).

Baldridge, K.K.; Cozzi, F.; Siegel, J.S.
Basicity (2,6-Pyridino)paracylcophanes: Lone-pair-π, Cation-π, and Solvation Effects,
Angewandte Chem. Int. Ed., VIP article, 51, 2103 (**2012**).

Abramson, R.; Baldridge, K. K.
Defined Sector Explicit Solvent in Continuum Model Approach for Computational Prediction of pKa,
Mol. Phys. (Festschrift Issue for Peter R Taylor), (**2012**).
DOI:10.1080/00268976.2012.687465

Zoppi, L.; Siegel, J.S.; Baldridge, K. K.
Electron Transport and Optical Properties of Curved Aromatics
WIREs, (**2012**). DOI: 10.1002/wcms.1107

Ni, L.; Baldridge, K.; Patzke, G.R.
New Polyoxometalate Catalysts: Switching the Way to Homogeneous Alcohol Oxidation
Chem. Eur. J., in press (**2012**).

Bauert, T.; Zoppi, L.; Siegel, J.S.; Baldridge, K.K.; Ernst, K.-H.
Pentagonal tiling with buckybowls: Pentamethylcorannulene on Cu(111),
Phys. Chem. Chem. Phys., (**2012**). DOI: 10.1039/c2cp41732d

King, B. T.; Olmstead, M.M.; Baldridge, K.K.; Kumar, B.; Balch, A.L.; Gharamaleki, J.A.
Molecular nesting in co-crystals of tetrabenzoquadrannulene and C60,
ChemComm, (**2012**). DOI:10.1039/c2cc34472F

Group of Christophe Copéret
Laboratory of Inorganic Chemistry
ETH Zürich

www.coperetgroup.ethz.ch

Areas of Research:

Surface and Interfacial Chemistry

The group of Surface and Interfacial Chemistry aims at the molecular understanding of the structure and the chemistry of oxide and metal surfaces by combining advanced spectroscopic methods and computational chemistry with the goal to generate single-site catalysts and supported nanoparticles, where the structure and the interface between the metal and the support are controlled at the molecular level.

References

R. Wischert, P. Laurent, C. Copéret, F. Delbecq, and P. Sautet,
γ-Alumina: the Essential and Unexpected Role of Water for the Structure, Stability, and Reactivity of "Defect" Sites.
J. Am. Chem. Soc. Just Accepted Manuscript DOI: 10.1021/ja3042383 (**2012**).

R. Kerber, A. Kermagoret, E. Callens, P. Florian, D. Massiot, A. Lesage, C. Copéret, F. Delbecq, X. Rozanska, P. Sautet ,
Nature and structure of aluminum surface sites grafted on silica from a combination of high field aluminum-27 solid-state NMR spectroscopy and first principle calculations
J. Am. Chem. Soc. 134, 6767 (**2012**).

R. Wischert, C. Copéret, F. Delbecq, P. Sautet,
Dinitrogen: a selective probe for tri-coordinate Al “defect” sites on alumina.
Chem. Commun., 47, 4890 (**2011**).

R. Wischert, C. Copéret, F. Delbecq, P. Sautet,
Optimal water coverage on alumina: a key to generate Lewis acid-base pairs reactive towards the C-H bond activation of methane.
Angew. Chem. Int. Ed., 50, 3202 (**2011**).

Group of Alessandro Curioni
IBM Research – Zurich Research Laboratory

www.zurich.ibm.com/mcs/compsci/

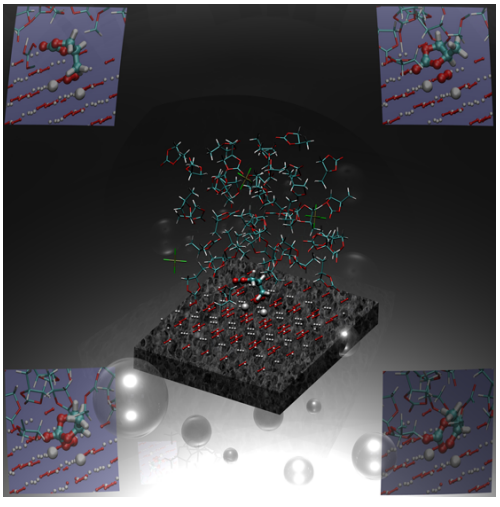
Areas of Research:

Simulation of complex systems in material sciences and biochemistry, parallel computing.

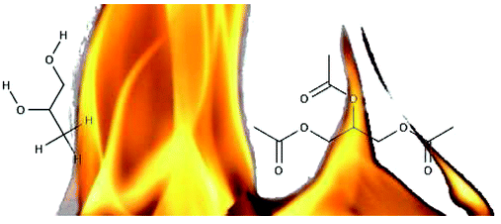
Keywords:

Computational sciences, multiscale simulations, density functional theory and applications, algorithms re-engineering for massively parallel computers, simulations for energy storage and conversion.

Main research topics:



(a) Simulation of chemical processes at complex interfaces in Li/Air batteries



(b) Simulation of pyrolitic decomposition of organic molecules

References

L Gross, F Mohn, N Moll, B Schuler, A Criado, E Guitián, D Peña, A Gourdon, Gerhard Meyer
Bond-Order Discrimination by Atomic Force Microscopy
Science 337 (6100), 1326-1329 (**2012**)

Yves Ineichen, Andreas Adelmann, Costas Bekas, Alessandro Curioni, Peter Arbenz
A fast and scalable low dimensional solver for charged particle dynamics in large particle accelerators
Computer Science – Research and Development 5, (**2012**)

G. Shumkin, F. Zipoli, A. Popov, A. Curioni
Multiscale Quantum Simulation of Resistance Switching in Amorphous Carbon *Procedia Computer Science* 9, 641-650 (**2012**)

N. Moll, L .Gross, F. Mohn, A. Curioni, G. Meyer
A simple model of molecular imaging with noncontact atomic force microscopy
New Journal of Physics 14 (8), 083023 (**2012**)

F. Mohn, L. Gross, N. Moll, G. Meyer
Imaging the charge distribution within a single molecule
Nature nanotechnology 7 (4), 227-231 92012)

P. Shemella, T. Laino, O. Fritz, A. Curioni
Understanding the Self-Healing Hydrophobic Recovery of High-Voltage Insulators
The Journal of Physical Chemistry B 116 (24), 7351-7356 (**2012**)

A .Fuhrer, F.Rueß, N. Moll, A. Curioni, D .Widmer
Atomic structure of Mn wires on Si (001) resolved by scanning tunneling microscopy
Physical Review Letters (in press) arXiv preprint arXiv:1205.0466 (**2012**)

T. Laino, C. Tuma, P. Moor, E. Martin, S. Stolz, A. Curioni
Mechanisms of Propylene Glycol and Triacetin Pyrolysis
The Journal of Physical Chemistry A 116 (18), 4602-4609 (**2012**)

T Laino, A Curioni
A New Piece in the Puzzle of Lithium/Air Batteries: Computational Study on the Chemical Stability of Propylene Carbonate in the Presence of Lithium Peroxide
Chemistry-A European Journal 18 (12), 3510-3520 (**2012**)

C Bekas, A Curioni, P Arbenz, C Flaig, GH van Lenthe, R Müller, AJ Wirth
Massively Parallel Graph Partitioning: A Case in Human Bone Simulations
Combinatorial Scientific Computing 12, 407 (**2012**)

Y. Ineichen, A. Adelmann, C. Bekas, A. Curioni, P. Arbenz
Computer Science-Research and Development, 1-8 1 (**2012**)

Valéry Weber and D. Asthagiri
Regularizing Binding Energy Distributions and the Hydration Free Energy of Protein Cytochrome C from All-Atom Simulations
J. Chem. Theory Comput., 2012, 8 (9), pp 3409–3415

H Freedman, T Laino, A Curioni
Reaction dynamics of ATP hydrolysis in actin determined by ab initio molecular dynamics simulations
Journal of Chemical Theory and Computation, in press (**2012**)

P. Khomyakov, W. Andreoni, N. Afify, A. Curioni
Large-Scale Simulations of a-Si: H: The Origin of Midgap States Revisited
Physical Review Letters 107 (25), 25550 (**2011**)

W. Andreoni, A. Curioni, J. Kroes, F. Pietrucci, O. Gröning
Exohedral Hydrogen Chemisorption on a Carbon Nanotube: The Clustering Effect
The Journal of Physical Chemistry C 116 (1), 269-275 (**2011**)

P. Shemella, T. Laino, O. Fritz, A. Curioni
"Surface Dynamics of Amorphous Polymers Used for High-Voltage Insulators:
The Journal of Physical Chemistry B 115 (46), 13508-13512 (**2011**)

L Gross, N Moll, F Mohn, A Curioni, G Meyer, F Hanke, M Persson
High-resolution molecular orbital imaging using a p-wave STM tip
Physical review letters 107 (8), 86101 (**2011**)

C Bekas, A Curioni, I Fedulova
Low-cost data uncertainty quantification
Concurrency and Computation: Practice and Experience 24 (8), 908-920 (**2011**)

G. Shumkin, A. Popov, A. Curioni, T. Laino
Ab initio simulation of a molecular switch on the base of an isomerization reaction
Mathematical Models and Computer Simulations 3 (3), 375-381 (**2011**)

T. Laino, C. Tuma, A. Curioni, E. Jochnowitz, S. Stolz
A Revisited Picture of the Mechanism of Glycerol Dehydration
The Journal of Physical Chemistry A 115 (15), 3592-3595 (**2011**)

M. Bokdam, P. A. Khomyakov, G. Brocks, P. J. Kelly
Electrostatic doping of graphene through ultrathin hexagonal boron nitride films.
Nano Letters 11, 4631 (**2011**)

Group of Ive Hermans
Institute of Chemical and Bioengineering
ETH Zürich

www.hermans.ethz.ch

Areas of Research:

Sustainable Chemistry and Catalysis

Keywords:

DFT, transition state theory (TST), selective oxidations, chemical kinetics, renewable substrates

References

U. Neuenschwander, I. Hermans,
The Conformations of Cyclooctene: Consequences for Epoxidation Chemistry
Journal of Organic Chemistry 76, 10236-10240, (**2011**).

C. Aellig, U. Neuenschwander, I. Hermans,
Acid-Catalyzed Decomposition of the Benzyl-Nitrite Intermediate during the HNO3-Mediated Aerobic Oxidation of Benzyl Alcohol
ChemCatChem, 4, 525-529, (**2012**).

U. Neuenschwander, B. Czarniecki, I. Hermans,
The Origin of Regioselectivity in Humulene Functionalization
Journal of Organic Chemistry, 77, 2865–2869, (**2012**).

U. Neuenschwander, E. Meier, I. Hermans,
Catalytic Epoxidations with Peroxides: Molybdenum Trioxide Species as the Origin of Allylic By-Products
Chemistry a European Journal, 18, 6776-6780, (**2012**)
(highlighted in Chimia, 7-8, 643, (**2012**)).

M. T. Schümperli, C. Hammond, I. Hermans,
Reactivity of Alpha-Amino-Peroxyl Radicals and Consequences for Amine Oxidation Chemistry
Physical Chemistry Chemical Physics, 14, 11002-11007, (**2012**).

Group of Philippe H. Hünenberger
Laboratory of Physical Chemistry
ETH Zürich

www.csms.ethz.ch

Areas of Research:

Computer simulation of molecular systems

Keywords:

Computer simulation, molecular dynamics, method development, force field, electrostatics, boundary conditions, conformational sampling, free-energy calculations, ionic systems, (bio)molecular systems

Main research topics:

The research of our group focuses on the development and application of methods for the *classical computer simulation of molecular systems*, namely in terms of *method development* :

- Treatment of electrostatic interactions
- Force-field parametrization (GROMOS)
- Thermodynamic boundary conditions
- Enhanced conformational sampling
- Extended-system methods
- Free-energy calculations
- Development of simulation algorithms
- Development of trajectory analysis methods

and in terms of *applications* :

- Single-ion solvation (book: www.csms.ethz.ch/single_ion_solvation)
- Properties of ionic systems (electrolyte solutions, crystals)
- Simulation of biomolecular systems (with a main focus on carbohydrates and lipids)
- Role of electrostatic interactions (hydrogen bonding, salt bridges) in (bio)molecular systems

References

H.S. Hansen, P.H. Hünenberger,
A reoptimized GROMOS force field for hexopyranose-based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers and glycosidic linkage conformers,
J. Comput. Chem., 32, 998-1032 (**2011**)

M.M. Reif, P.H. Hünenberger,
Computation of methodology-independent single-ion solvation properties from molecular simulations. III. Correction terms for the solvation free energies, enthalpies, entropies, heat capacities, volumes, compressibilities and expansivities of solvated ions,
J. Chem. Phys., 134, 144103/1-144103/30 (**2011**)

M.M. Reif, P.H. Hünenberger,
Computation of methodology-independent single-ion solvation properties from molecular simulations. IV. Optimised Lennard-Jones interaction parameter sets for the alkali and halide ions in water,
J. Chem. Phys., 134, 144104/1-144104/25 (**2011**)

B. Keller, P.H. Hünenberger, W.F. van Gunsteren,
An analysis of the validity of Markov state models for emulating the dynamics of classical molecular systems and ensembles,
J. Chem. Theory Comput., 7, 1032-1044 (**2011**)

B.A.C. Horta, P.F.J. Fuchs, W.F. van Gunsteren, P.H. Hünenberger,
New interaction parameters for oxygen compounds in the GROMOS force field: Improved pure-liquid and solvation properties for alcohols, ethers, aldehydes, ketones, carboxylic acids and esters,
J. Chem. Theory Comput., 7, 1016-1031 (**2011**)

B.A.C. Horta, P.H. Hünenberger,
Enantiometic segregation in the gel phase of lipid bilayers,
J. Am. Chem. Soc., 133, 8464-8465 (**2011**)

P. Hünenberger, M. Reif,
Single-Ion Solvation. Experimental and Theoretical Approaches to Elusive Thermodynamic Quantities,
Authored book, RSC Theoretical and Computational Chemistry Series (**2011**)

A. Choutko, W.F. van Gunsteren, P.H. Hünenberger,
Preferential affinity of the components of liquid mixtures at a rigid non-polar surface: Enthalpic and entropic driving forces,
Chem. Phys. Chem., 12, 3214-3223 (**2012**)

S. Riniker, C.D. Christ, H.S. Hansen, P.H. Hünenberger, C. Oostenbrink, D. Steiner, W.F. van Gunsteren,
Calculation of relative free energies for ligand-protein binding, solvation and conformational transitions using the GROMOS software,
J. Phys. Chem. B, 115, 13570-13577 (**2012**)

S. Riniker, B.A.C. Horta, B. Thijssen, S. Gupta, W.F. van Gunsteren, P.H. Hünenberger,
Temperature dependence of the dielectric permittivity of acetic acid, propionic acid and their methyl esters: A molecular dynamics simulation study,
Chem. Phys. Chem., 13, 1182-1190 (**2012**)

A.-P.E. Kunz, N. Schmid, S. Riniker, J.R. Allison, B.A.C. Horta, D.J. Geerke, P.H. Hünenberger, W.F. van Gunsteren,
New functionalities in the GROMOS biomolecular simulation software,
J. Comput. Chem., 33, 340-353 (**2012**)

B.A.C. Horta, Z. Lin, W. Huang, W.F. van Gunsteren, P.H. Hünenberger,
Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: Influence on the folding properties of two beta-peptides in methanol,
J. Comput. Chem., 33, 1907-1917 (**2012**)

M.M. Reif, P.H. Hünenberger, C. Oostenbrink,
New interaction parameters for charged amino acid side chains in the GROMOS force field,
J. Chem. Theory Comput., in press (**2012**)

B. Dahlgren, M.M. Reif, P.H. Hünenberger, N. Hansen,
Calculation of derivative thermodynamic hydration and aqueous partial molar properties of ions based on atomistic simulations,
J. Chem. Theory Comput., in press (**2012**)

P.F.J. Fuchs, H.S. Hansen, P.H. Hünenberger, B.A.C. Horta,
A GROMOS parameter set for vicinal diether functions: properties of polyethyleneoxide and polyethyleneglycol,
J. Chem. Theory Comput., in press (2012)

Group of Jürg Hutter
Physical Chemistry Institute
University of Zürich

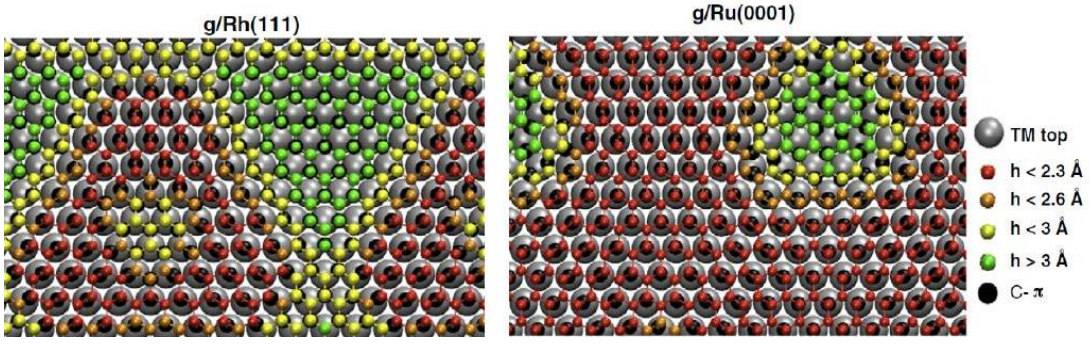
www.pci.uzh.ch

Areas of Research:

Method development and applications of ab initio molecular dynamics, molecules at interfaces (solid/liquid, liquid/vapor), chemical reactions in solution

Keywords:

Electronic structure theory, molelcular dynamics, density functional theory, condesned phase, interfaces, liquids, solutions, chemical reactions



Top view of the Moire superstructure formed by 12x12 g over 11x11 Ru(0001) and Rh(111). The gray spheres are the metal atoms of the topmost layer of the slab. The C atoms of the overlayer are colored according to distance from the substrate. Red are C closer than 2.3 Åorange are C between 2.3 and 2.6 Åyellow between 2.6 and 3 Åand green above 3 ÅThe black spheres represent the centers of the C-π MLWO.

References

J. Hutter,
Car-Parrinello molecular dynamics,
Wiley Interdisciplinary Reviews: Comp. Mol. Sci. 2 604-612 (**2012**)

Barbara Kirchner, Philipp J di Dio, Jürg Hutter,
Real-world predictions from ab initio molecular dynamics simulations,
Topics in current chemistry 307, 109 (**2012**)

Fabien Devynck, Marcella Iannuzzi and Matthias Krack,
Frenkel pair recombinations in UO2: Importance of explicit description of polarisability in core-shell molecular dynamics simulations,
Phys. Rev. B 85 183103 (**2012**)

H. Enriquez, A. Mayne, A. Kara, S. Vizzini, S. Roth, B. Lalmi, A. P Seitsonen, B. Aufray, T. Greber, R. Belkhou, G. Dujardin and H. Oughaddou, Adsorption of silicon on Au(110): An ordered two dimensional surface alloy,
Applied Physics Letters 101 021605 (**2012**)

J.-L. Valla-Pardo, M. Guijt, M. Iannuzzi, K. S Joya, H J M de Groot and F. Buda,
Ab initio molecular dynamics study of water oxidation reaction pathways in mono-Ru catalysts,
ChemPhysChem 13 140-146 (**2012**)

Konstanze R Hahn, Antonio Tricoli, Gianluca Santarossa, Angelo Vargas and Alfons Baiker,
First-principles analysis of H2O adsorption on the (110) surfaces of SnO2, TiO2 and their solid solutions,
Langmuir 28 1646-1656 (**2012**)

S. Vijayaraghavan, D. Ecija, W. Auwärter, S. Joshi, K. Seufert, A. P Seitsonen, K. Tashiro and J. V Brth,
Selective supramolecular fullerene-porphyrin interactions and switching in surface-confined C60-Ce(TPP)2 dyads,
Nano Letters, 12 4077 (**2012**)

A. S Pensado, M. Brehm, J. Thar, A. P Seitsonen and B. Kirchner,
Effect of dispersion on the structure and dynamics of the ionic liquid 1-ethyl-3-methylimidazolium thiocyanate,
ChemPhysChem 13 1845-1853 (**2012**)

A. C Papageorgiou, S. Fischer, J. Reichert, K. Diller, F. Blobner, F. Klappenberger, F. Allegretti, A. P Seitsonen and J. V Barth,
Chemical transformations drive complex self-assembly of uracil on close-packed coinage metal surfaces,
ACS Nano 6 2477-2486 (**2012**)

F. Hess, A. Farkas, Ari P Seitsonen and H. Over,
"First-Principles" kinetic monte carlo simulations revisited: CO oxidation over RuO2(110),
J. Comp. Chem. 33 757-766 (**2012**)

Y. Makoudi, E. Arras, N. Kepcija, W. Krenner, S. Klyatskaya, F. Klappenberger, M. Ruben, Ari P Seitsonen and J. V Barth,
A Hierarchically Organised Bimolecular Ladder-Network Exhibiting Guided One-Dimensional Diffusion,
ACS Nano 6 549-556 (**2012**)

J. P Hofmann, S. F Rohrlack, F. Hess, J. C Goritzka, P. P T Krause, Ari P Seitsonen, W. Moritz and H. Over,
Adsorption of chlorine on Ru(0001): A combined density functional theory and quantitative low energy electron diffraction study,
Surface Science 606 297-304 (**2012**)

M. Salanne, L. J A Siqueira, Ari P Seitsonen, P. A Madden and B. Kirchner,
From molten salts to room temperature ionic liquids: Simulation studies on chloroaluminate systems,
Faraday Discussions 154 171-188 (**2012**)

A. Kara, H. Enriquez, Ari P Seitsonen, LC Lew Yan Voon, S. Vizzini, B. Aufray and H. Oughaddou,
A review on silicene - New candidate for electronics,
Surface Science Reports 67 1-18 (**2012**)

Edit Matyus, Jürg Htter, Ulrich Müller-Herold and Markus Reiher,
Extracting elements of molecular structure from the all-particle wave function,
J. Chem. Phys. 135, 204302 (**2011**)

Yun Ding, Iannuzzi Marcella and Jürg Htter,
Investigation of Boron Nitride Nanomesh Interacting with Water,
J. Phys. Chem. C 115, 13685-13692 (**2011**)

Marcella Iannuzzi and Jürg Htter,
Comparative study of the nature of chemical bonding of corrugated graphene on Ru(0001) and Rh(111) by electronic structure calculations,
Surface Science 605, 1360-1368 (**2011**)

Garold Murdachaew, Christopher J Mundy, Gregory K Schenter, Teodoro Laino and Jürg Htter,
Semiempirical Self-Consistent Polarization Description of Bulk Water, the Liquid-Vapor Interface, and Cubic Ice,
J. Phys. Chem. A 115, 6046-6053 (**2011**)

Edit Matyus, Jürg Htter, Ulrich Müller-Herold and Markus Reiher,
On the emergence of molecular structure,
Phys. Rev. A 83, 052512 (**2011**)

Yun Ding, Iannuzzi Marcella and Jürg Htter,
Investigation of h-BN/Rh(111) Nanomesh Interacting with Water and Atomic Hydrogen,
Chimia 65, 256-259 (**2011**)

Hiroko Satoh, Shino Manabe, Yukishige Ito, Hans P Lüthi, Teodoro Laino and Jürg Htter,
Endocyclic Cleavage in Glycosides with 2,3-trans Cyclic Protecting Groups,
J. Am. Chem. Soc. 133, 5610-5619 (**2011**)

Marie-Laure Bonnet and Vincent Tognetti,
The influence of density functional approximations on the description of LiH + NH3 -> LiNH2 + H2 reaction,
Chem. Phys. Lett. 511 427-433 (**2011**)

Romain Jonchiere, Ari P Seitsonen, Guillaume Ferlat, A Marco Saitta and Rodolphe Vuilleumier,
Van der Waals effects in ab initio water at ambient and supercritical conditions,
J. Chem. Phys. 135, 154503 (**2011**)

Laura E Oikkonen, Maria G Ganchenkova, Ari P Seitsonen and Risto M Nieminen,
Vacancies in CuInSe2: New insights from hybrid-functional calculations,
Journal of Physics: Condensed Matter 23, 422202 (**2011**)

Mauro Del Ben, Remco W A Havenith, Ria Broer and Mauro Stener,
Density Functional Study on Morphology and Photoabsorption of CdSe Nanoclusters,
J. Phys. Chem. C 115, 16782-16796 (**2011**) F. Rossel, M. Pivetta, F. Patthey, E. Cavar, A. P Seitsonen and Wolf-Dieter Schneider,
Growth and characterization of fullerene nanocrystals on NaCl/Au(111),
Phys. Rev. B 84 075426 (**2011**)

Group of Martin Quack
Laboratory of Physical Chemistry
ETH Zurich

www.ir.ethz.ch

Areas of Research:

Molecular Kinetics and Spectroscopy

Keywords:

Molecular Kinetics, Spectroscopy, Parity Violation, Chiral Molecules, Quantum Dynamics, Fundamental Symmetries, Quantum Chemical Kinetics, Tunneling, Infrared Spectroscopy, Terahertz Spectroscopy, Atmospheric Spectroscopy, Methane, Astrophysical Spectroscopy.

The group "Molecular Kinetics and Spectroscopy"of Martin Quack at ETH has as main research theme the understanding of fundamental, physical-chemical molecular primary processes. The basic research question concerns the fully quantum mechanical molecular motion, which is at the origin of all chemical reactions. An essential aspect of the research is the systematic combination of experimental and theoretical studies. The experimental studies concentrate on high resolution infrared spectroscopy, infrared multiphoton excitation and time resolved kinetic spectroscopy. While most of the experiments address fundamental questions, some practical applications relate to atmospheric and astrophysical spectroscopy and to isotope separation. The theory covers full-dimensional quantum dynamics by discrete variable representation techniques, finite basis set representation as well as diffusion quantum Monte Carlo methods. Approximate theories are developed and tested in relation to exact theories (an example is the quasiadiabatic channel reaction path hamiltonian theory for tunneling reactions). Another focus of theory is the time dependent quantum dynamics in intramolecular energy flow and vibrational redistribution, coherent infrared multiphoton excitation and laser chemistry as well as time dependent quantum statistical mechanical approaches to these processes. Finally, the group studies fundamental symmetry principles in molecular processes and molecular chirality in relation to parity violation. Our theoretical developments have led to large increases in the predicted parity violating energy differences between enantiomers, making these now a realistic goal for our current experiments.

References

S. Albert, K. Keppler Albert, P. Lerch, M. Quack
Highest resolution Fourier transform infrared (FTIR) spectroscopy of polyatomic molecules with and without synchrotron radiation in Proceedings of the 18th Symposium on Atomic, Cluster and Surface Physics 2012 (SASP 2012), Alpe d'Huez, France, 22 to 27 January 2012, pages 86 - 89, (Marius Lewerenz, Odile Dutuit, and Roberto Marquardt eds.,
Innsbruck University Press (IUP), Innsbruck, (**2012**),
ISBN 978-3-902811-42-4.

E. Miloglyadov, R. Prentner, G. Seyfang, M. Quack,
Inversion tunneling in normal and substituted anilines from infrared spectroscopy and quasiadiabatic channel reaction path Hamiltonian calculations
in Proceedings of the 18th Symposium on Atomic, Cluster and Surface Physics 2012 (SASP 2012), Alpe d'Huez, France, 22 to 27 January 2012, pages 234 - 237, (Marius Lewerenz, Odile Dutuit, and Roberto Marquardt eds.,
Innsbruck University Press (IUP), Innsbruck, (**2012**),
ISBN 978-3-902811-42-4.

P. Dietiker, M. Quack, A. Schneider, G. Seyfang, and F. Ünlü
IR-laser induced population transfer from highly populated rotational levels of NH_3 in a molecular beam in Proceedings of the 18th Symposium on Atomic, Cluster and Surface Physics 2012 (SASP 2012), Alpe d'Huez, France, 22 to 27 January 2012, pages 263 - 267, (Marius Lewerenz, Odile Dutuit, and Roberto Marquardt eds.,
Innsbruck University Press (IUP), Innsbruck, (**2012**),
ISBN 978-3-902811-42-4.

Ph. Lerch, P. Dumas, T. Schilcher, A. Nadji, A. Luedeke, N. Hubert, L. Cassinari, M. Boege, J.-C. Denard, L. Stingelin, L. Nadolski, T. Garvey, S. Albert, C. Gough, M. Quack, J. Wambach, M. Dehler and J. M. Filhol,
Assessing noise sources at synchrotron infrared ports
J. Synchrotron Rad. 19, 1 - 9 (**2012**).

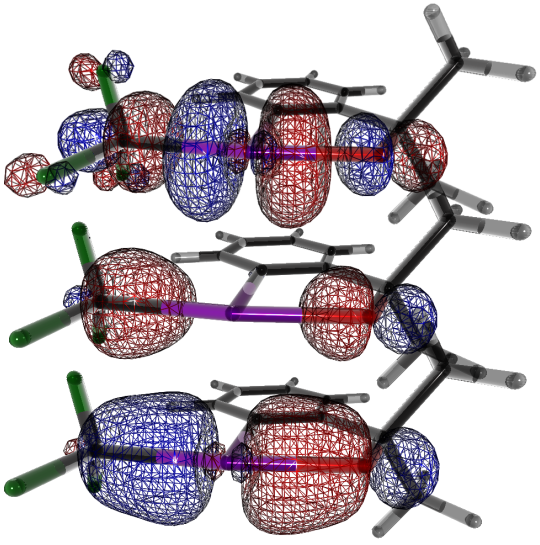
C. Manca Tanner, M. Quack
Reinvestigation of the $\nu_2 + \nu_2\nu_3$ subband in the overtone icosad of $^{12}CH_4$ using cavity ring-down (CRD) spectroscopy of a supersonic jet expansion
Mol. Phys. 110, 2111 - 2135 (**2012**).

T. P. Softley V. Boudon, P. De Natale, M. Herman, M. Quack,
Foreword: 22nd Colloquium on High Resolution Molecular Spectroscopy Dijon 29 August to 2 September 2012
Mol. Phys. 110, 2001 - 2001 (**2012**).

M. Quack,
Molecular Parity Violation and Chirality: The Asymmetry of Life and the Symmetry Violations of Physics in Quantum Systems in Chemistry and Physics: Progress in Methods and Applications, Proceedings of QSCP XVI, Kanazawa 11 to 17 September 2011, Series Title: Progress in Theoretical Chemistry and Physics, (Kiyoshi Nishikawa; Jean Maruani; Erkki Brändas; Gerardo Delgado-Barrio;
Piotr Piecuch Eds., Springer Verlag (**2012**), pages 47 - 76.

Group of Hans P. Lüthi
Laboratory of Physical Chemistry
ETH Zurich

www.luethi.ethz.ch



Representation of the localized (NBO)
3-center-4-electron bond in Togni's reagent

Areas of Research:

Electronic Structure Theory and Applications, Computational Science

Keywords:

Quantum chemistry, chemical bonding, quantitative structure-property relationships (QSPR), chemical reactivity; wave function theory, density functional theory, data processing, data analysis

References

H. Satoh, S. Manabe, Y. Ito, H.P. Lüthi, T. Laino and J. Hutter,
Endocyclic Cleavage in Glycosides with 2,3-trans Cyclic Protecting Groups,
J. Am. Chem. Soc., 133, 5610-5619 (**2011**)

P.A. Limacher and H.P. Lüthi,
Cross Conjugation,
Wiley Interdisciplinary Reviews (WIRE), issue on Computational Molecular Science (by invitation), Volume 1 (**2011**)

P.A. Limacher, Q. Li and H.P. Lüthi,
On the effect of electron correlation on the static second hyperpolarizability of π conjugated oligomer chains
J. Chem. Phys. 135, 014111 (**2011**)

H. Pinto de Magalhães, H.P. Lüthi and A. Togni,
Reductive Eliminations from lambda(3)-Iodanes: Understanding Selectivity and the Crucial Role of the Hypervalent Bond
Org. Lett., 14, 3830-3833 (**2012**)

A. Glöss, M.P. Brändle, W. Klopper and H.P. Lüthi,
The MP2 binding energy of the ethene dimer and its dependence on the auxiliary basis sets: a benchmark study using a newly developed infrastructure for the processing of quantum chemical data
Mol. Phys., in press (DOI: 10.1080/00268976.2012.708793)

Group of Reinhard Nesper
Laboratory of Inorganic Chemistry
ETH Zurich

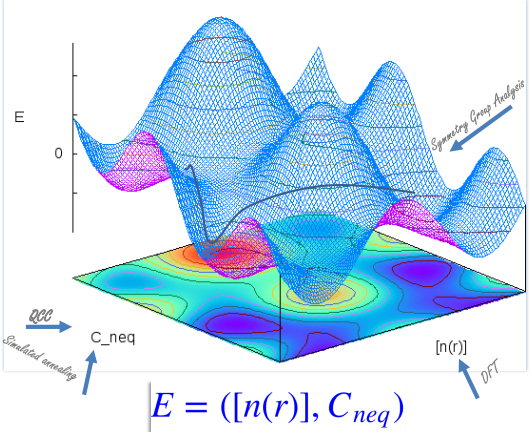
www.solid.ethz.ch

Areas of Research:

Crystal structure prediction, Enthalpy of formation, Electronic Structure calculations

Keywords:

Simulated Annealing, DFT total energy calculations, Symmetry group analysis and representation



The concept of inorganic crystal structure prediction from a complete first-principles approach, by using the chemical formula as the sole starting knowledge, is still a challenging task. Several methodologies have been proposed and adopted along decades, adapting them to specific systems under study. Our methodology combines Quantum Chemistry Cluster calculations (QCC), Simulated Annealing optimization (SA) [2], total energy calculations via DFT, and Symmetry Group Relations (SGR) [3] to explore the Potential Energy Surface of a system. Depending on whether we search for structural transformations of a system with a given stoichiometry, or study absorption processes, the atomic ratio can be a constant or a variable, respectively, but in both cases the final target is the identification of the ground-state and local minima. The case studies are represented by complex borohydrides (1), in particular $\mathrm{LiBH_x}, x \leq 4$, and $\mathrm{Mg(BH_4)_2}$ (2). For $\mathrm{LiBH_x}, x = 2$ (3), the predicted lowest energy structure shows the formation of anionic linear chains.

[2] in collaboration with Prof A. Tekin, Istanbul Technical University.

[3] in collaboration with Prof W. Sikora, AGH University of Science and Technology, Cracow

References

R. Caputo, A. Tekin,
Ab-initio crystal structure prediction. A case study: $\mathrm{NaBH_4}$,
J. Solid State Chem., 184, 1622 (**2011**)

R. Caputo, A. Kupczak, W. Sikora, and A. Tekin,
Ab-initio crystal structure prediction by combining symmetry analysis representation and total energy calculations. An insight into the structure of $\mathrm{Mg(BH_4)_2}$,
Phys. Chem. Chem. Phys., (**submitted**)

R. Caputo, A. Tekin,
Lithium dihydroborate. First-principles structure prediction of $\mathrm{LiBH_2}$,
Inorg.Chem., 51, 9757 (**2012**)

Group of M. Parrinello

Department of Chemistry and Applied Biosciences, ETH Zürich
&
Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana

www.rgp.ethz.ch

Areas of Research:

Computer Simulations of Materials and Biomolecules

Keywords:

Ab-initio molecular dynamics, enhanced sampling methods, collective variables, nucleation, phase change materials, hydrogen bonded systems, ligand protein interaction, large motions in proteins and RNA.

References

A. Barducci, M. Bonomi and M. Parrinello,
Metadynamics,
Comp. Mol. Sci., 1, 826-843 (**2011**)

G. A. Tribello, J. Cuny, H. Eshet and M. Parrinello,
Exploring the free energy surfaces of clusters using reconnaissance metadynamics,
J. Chem. Phys., 135 (11), 114109 (**2011**)

C. S. Cucinotta, M. Bernasconi and M. Parrinello,
Hydrogen Oxidation Reaction at the Ni/YSZ Anode of Solid Oxide Fuel Cells from First Principles,
Phys. Rev. Lett., 107 (20), 206103 (**2011**)

A. Hassanali, M. K. Prakash, H. Eshet and Michele Parrinello,
On the recombination of hydronium and hydroxide ions in water,
PNAS, 108 (51), 20410-20415 (**2011**)

A. Berteotti, A. Barducci and Michele Parrinello,
Effect of Urea on the β-Hairpin Conformational Ensemble and Protein Denaturation Mechanism,
J. Am. Chem. Soc., 133, 17200-17206 (**2011**)

V. Limongelli, L. Marinelli, S. Cosconati, C. La Motta, S. Sartini, L. Mugnaini, F. Da Settimo, E. Novellino and M. Parrinello,
Sampling protein motion and solvent effect during ligand binding,
PNAS, 109 (5), 1467-1472 (**2012**)

G. Grazioso, V. Limongelli, D. Branduardi, E. Novellino, C. De Micheli, A. Cavalli and M. Parrinello,
Investigating the Mechanism of Substrate Uptake and Release in the Glutamate Transporter Homologue Glt(Ph) through Metadynamics Simulations,
J. Am. Chem. Soc., 134 (1), 453-463 (**2012**)

H. Eshet, R. Z. Khaliullin, T. D. Kühne, J. Behler and M. Parrinello,
Microscopic Origins of the Anomalous melting Behavior of Sodium under High Pressure,
Phys. Rev. Lett. 108, 115701 (**2012**)

G. A. Tribello, M. Ceriotti and M. Parrinello,
Using sketch-map coordinates to analyze and bias molecular dynamics simulations,
PNAS, 109 (14), 5196-5201 (**2012**)

P. Söderhjelm, G. A. Tribello and M. Parrinello,
Locating binding poses in protein-ligand systems using reconnaissance metadynamics,
PNAS, 109 (14), 5170-5175 (**2012**)

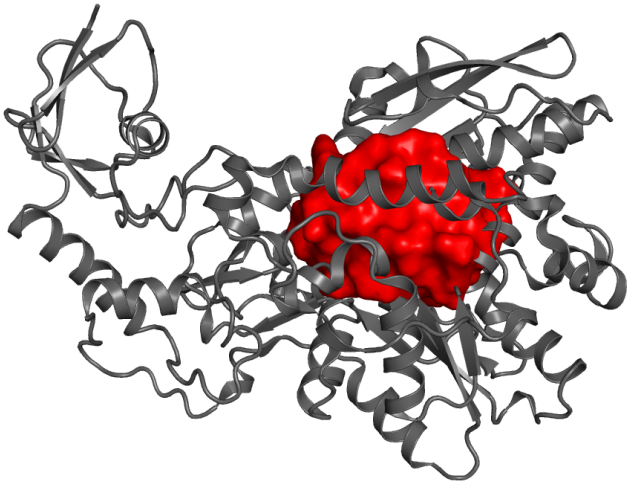
A. A. Hassanali, J. Cuny, M. Ceriotti, C. J. Pickard and M. Parrinello,
The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates,
J. Am. Chem. Soc., 134, 8557-8569 (**2012**)

D. Munoz-Santiburcio, M. Kosa, A. Hernandez-Laguna, C. I. Saint-Diaz and M. Parrinello,
Ab Initio Molecular Dynamics Study of the Dehydroxylation Reaction in a Smectite Model,
Phys. Chem. C, 116, 12203-12211 (**2012**)

D. Branduardi, G. Bussi and Michele Parrinello,
Metadynamics with Adaptive Gaussians,
J. Chem. Theory Comput. 8, 2247-2254 (**2012**)

Group of Markus Reiher
Laboratory of Physical Chemistry
ETH Zurich

www.reiher.ethz.ch



Cartoon representation of [FeFe] hydrogenase crystal structure[4].
In red highlighted the extended model of the enzyme active site (700 atoms).

Synopsis:

Our research concentrates on theory in chemistry with a special emphasis on so-called first-principles methods, which are deeply rooted in quantum mechanics.

Areas of Research:

Relativistic Quantum Chemistry and Atomic Physics, Electron-Electron Interaction – DMRG and DFT, Theoretical Bio-Inorganic Chemistry and Coordination Chemistry, Quantum Chemical Analysis of Novel Compounds, Vibrational Spectroscopy of Large Molecules

Keywords:

Relativistic Quantum Chemistry and Atomic Physics; Electron-Electron Interaction – DMRG, TNS, and DFT; Theoretical Bio-Inorganic Chemistry and Coordination Chemistry; Quantum Chemical Analysis of Novel Compounds; Vibrational Spectroscopy of Large Molecules; Haptic Quantum Chemistry

[4] PDB entry 3C8Y: A.S. Pandey et.al., *J. Am. Chem. Soc.* (**2008**), 130, 4533.

References

M. K. Bruska, M. T. Stiebritz, M. Reiher,
Regioselectivity of H-Cluster Oxidation
J. Am. Chem. Soc., 133, 20588 (**2011**)

E. Mátyus, J. Hutter, U. Müller-Herold, M. Reiher,
Extracting elements of molecular structure from the all-particle wave function
J. Chem. Phys., 135, 204302, (**2011**)

D. Peng, M. Reiher
Exact Decoupling of the Relativistic Fock Operator
Theor. Chem. Acc., 131, 1081 (**2012**)

D. Peng, M. Reiher
Local Relativistic Exact Decoupling
J. Chem. Phys., 136, 244108 (**2012**)

B. Simmen, T. Weymuth, M. Reiher,
How many Chiral Centers can Raman Optical Activity Spectroscopy Distinguish in a Molecule?
J. Phys. Chem. A, 116, 5410 (**2012**)

M. T. Stiebritz, M. Reiher,
Hydrogenases and Oxygen
Chem. Sci., 3, 1739 (**2012**)

K. Boguslawski, K. H. Marti, Ö. Legeza, M. Reiher,
Accurate ab initio spin densities
J. Chem. Theory Comput., 8, 1970 (**2012**)

T. Weymuth, M. P. Haag, K. Kiewisch, S. Luber, S. Schenk, Ch. R. Jacob, C. Herrmann, J. Neugebauer, M. Reiher,
MOVIPAC: Vibrational Spectroscopy with a Robust Meta-Program for Massively Parallel Standard and Inverse Calculations
J. Comput. Chem., 33, 2186 (**2012**)

E. Mátyus, M. Reiher,
Molecular Structure Calculations: A Unified Quantum Mechanical Description of Electrons and Nuclei Using Gaussian Functions and the Global Vector Representation
J. Chem. Phys., 137, 024104 (**2012**)

S. Fux, M. Reiher,
Electron Density in Quantum Theory
Struct. Bonding, 147, 99 (**2012**)

M. Reiher,
Relativistic Douglas-Kroll-Hess Theory
Wiley Interdisciplinary Reviews - Computational Molecular Science, 2, 139 (**2012**)

R. Prins, V. K. Palfi, M. Reiher,
Hydrogen Spillover to Nonreducible Supports
J. Phys. Chem. C, 116, 14274 (**2012**)

Group of Franziska Schoenebeck
Institute for Organic Chemistry
ETH Zürich

www.oci.uzh.ch/research/baldridge.html

Areas of Research:

Physical organic chemistry, computational and experimental chemistry

Research interests in the Schoenebeck group are in the area of physical organic chemistry. The emphasis is on understanding reactivity and mechanisms, ultimately seeking the design of new catalysts and the development of novel applications in organic, bioorganic and materials chemistry.

Keywords:

Reactivity, Design, Mechanisms, QM

References

M. Aufiero, F. Proutiere, F. Schoenebeck,
Redox Reactions in Palladium Catalysis: On the Accelerating and/or Inhibiting Effects of Copper and Silver Salt Additives in Cross-Coupling Chemistry Involving Electron-rich Phosphine Ligands
Angew. Chem. Int. Ed., 51, 7226, (**2012**).

E. Lyngvi, J. W. Bode, F.Schoenebeck,
A Computational Study of the Origin of Stereoinduction in NHC-Catalyzed Annulation Reactions of α,β-Unsaturated Acyl Azoliums
Chem. Sci., 3, 2346, (**2012**).

F. Proutiere, M. Aufiero, F. Schoenebeck,
"On the Reactivity and Stability of Dinuclear Pd(I) Complexes: Studies on the Active Catalytic Species, Insights on Precatalyst Activation and Deactivation and Application in Highly Selective Cross-Coupling Reactions
J. Am. Chem. Soc., 134, 606, (**2012**).

Y. Zou, C. Ding, L. Zhou, Z. Li, Q. Wang, F. Schoenebeck, A. Goeke,
Tandem crossed-dimerisation/oxonia-Cope sequence of different carbonyl compounds to homoallylic esters and lactones
Angew. Chem. Int. Ed., 51, 5647, (**2012**).

E. Cahard, F. Schoenebeck, J. Garnier, S. P. Y. Cutulic, S. Zhou, J. A. Murphy
Electron Transfer to Benzenes by Photoactivated Neutral Organic Electron Donors
Angew. Chem. Int. Ed. (**2012**), 51, 1.

Solvent Effect on Palladium-Catalyzed Cross Coupling Reactions and Implications on the Active Catalytic Species,
F. Proutiere, F. Schoenebeck,
Angew. Chem. Int. Ed., 50, 8192, (**2011**).

P. Anstaett, F. Schoenebeck,
Reductive Elimination of $ArCF_3$ from Bidentate Pd(II) Complexes - A Computational Study,
Chem. Eur. J., 17, 12340, (**2011**).

G. Jayamurugan, J.-P. Gisselbrecht, C. Boudon, F. Schoenebeck, W. B. Schweizer, B. Bernet, F. Diederich,
Expanding the chemical space for push-pull chromophores by non-concerted [2+2] and [4+2] cycloadditions: access to a highly functionalised 6,6-dicyanopentafulvene with an intense, low-energy charge-transfer band
Chem. Commun., 47 (15), 4520, (**2011**).

Groups of M. Troyer and P. Werner
Theoretische Physik
ETH Zürich

www.itp.phys.ethz.ch

Areas of Research:

Computational condesned matter physics and high performance computing

Keywords:

Computational physics, strongly correlated fermions, ultracold quantum gases, Bose Einstein condensation, quantum devices, quantum Monte Carlo methods, tensor network methods, computational provenance

Special highlights:

We have developed a density funtional theory for ultracold atomic quantum gases, and applied it tot he study of the phase diagram of fermionic atoms captured in an optical lattice. This new density functional allows to use quantum chemistry methods for quantum gases, where controlled high precision experiments are possible that can be used to test predictions by static, time dependent, and finite temperature DFT calculations [5]

[5] P.N. Ma, S. Pilati, X. Dai and M. Troyer, Density functional theory for atomic Fermi gases, *Nature Physics* 8, 601 (**2012**).

References

S. Fuchs, E. Gull, L. Pollet, E. Burovski, E. Kozik, T. Pruschke, M. Troyer
Thermodynamics of the 3D Hubbard model on approach to the Neel transition
Phys. Rev. Lett. 106, 030401 (**2011**)

E. Gull, A.J. Millis, A.I. Lichtenstein, A.N. Rubtsov, M. Troyer, P. Werner
Continuous-time Monte Carlo methods for quantum impurity models
Rev. Mod. Phys. 83, 349 (**2011**)

B. Bauer, L. D. Carr, A. Feiguin, J. Freire, S. Fuchs, L. Gamper, J. Gukelberger, E. Gull, S. Guertler, A. Hehn, R. Igarashi, S.V. Isakov, D. Koop, P.N. Ma, P. Mates, H. Matsuo, O. Parcollet, G. Pawlowski, J.D. Picon, L. Pollet, E. Santos, V.W. Scarola, U. Schollwöck, C. Silva, B. Surer, S. Todo, S. Trebst, M. Troyer, M.L. Wall, P. Werner, S. Wessel
The ALPS project release 2.0: Open source software for strongly correlated systems
J. Stat. Mech., P05001 (**2011**)

Kai-Yu Yang, E. Kozik, Xin Wang, M. Troyer
Diagrammatic Quantum Monte Carlo solution of the two-dimensional Cooperon-Fermion model
Phys. Rev. B 83, 214516 (**2011**)

Sebastian Fuchs, Emanuel Gull, Matthias Troyer, Mark Jarrell, Thomas Pruschke
Spectral properties of the three-dimensional Hubbard model
Phys. Rev. B 83, 235113 (**2011**)

D. Koop, E. Santos, P. Mates, H.T. Vo, P. Bonnet, B. Bauer, B. Surer, M. Troyer, D.N. Williams, J.E. Tohline, Juliana Freire, C.T. Silva
A Provenance-Based Infrastructure for Creating Executable Papers
Procedia Computer Science, 4 648 (**2011**)

Anders, Emanuel Gull, Lode Pollet, Matthias Troyer, Philipp Werner
Dynamical mean field theory for bosons
New J. Phys 13, 075013 (**2011**).

P. Corboz, S. R. White, G. Vidal, M. Troyer
Stripes in the two-dimensional t-J model with infinite projected entangled-pair states
Phys. Rev. B 84, 041108(R) (**2011**)

Jia-Wei Huo, Fu-Chun Zhang, Weiqiang Chen, M. Troyer and U. Schollwöck
Trapped Ultracold Bosons in Periodic Lattice Modulations
Phys. Rev. A 84, 043608 (**2011**)

E. Gull, P. Werner, S. Fuchs, B. Surer, T. Pruschke and M. Troyer,
Continuous-time Quantum Monte Carlo impurity solvers
Computer Physics Communications 182, 1078 (**2011**)

Philippe Corboz, Andreas M. Laeuchli, Karlo Penc, Matthias Troyer, Frederic Mila
Simultaneous dimerization and SU(4) symmetry breaking of 4-color fermions on the square lattice
Phys. Rev. Lett. 107, 215301 (**2011**)

M. Sentef, P. Werner, E. Gull, and A. Kampf
Superconductivity and Pairing Fluctuations in the Half-Filled Two-Dimensional Hubbard Model
Phys. Rev. Lett. 107, 126401 (**2011**)

M. Eckstein and P. Werner
Thermalization of a pump-excited Mott insulator
Phys. Rev. B 84, 035122 (**2011**)

M. Sentef, P. Werner, E. Gull and A. Kampf
Charge and spin criticality for the continuous Mott transition in a two-dimensional organic conductor
Phys. Rev. B 84,165133 (**2011**)

M. Eckstein and P. Werner
Damping of Bloch oscillations in the Hubbard model
Phys. Rev. Lett. 107, 186406 (**2011**)

P. Werner, M. Casula, T. Miyake, F. Aryasetiawan, A. J. Millis, and S. Biermann
Satellites and large doping- and temperature-dependence of electronic properties in hole-doped $BaFe_2As_2$
Nature Physics 8, 331 (**2012**)

R. Kovacik, P. Werner, K. Dymkowski and C. Ederer
Rubidium superoxide: a p-electron Mott insulator
Phys. Rev. B 86, 075130 (**2012**)

N. Tsuji, T. Oka, H. Aoki and P. Werner
Repulsion-to-attraction transition in correlated electron systems triggered by a monocycle pulse
Phys. Rev. B 85, 155124 (**2012**)

B. Surer, M. Troyer, P. Werner, A.M. Läuchli, TO. Wehling, A. Wilhelm, A. I. Lichtenstein
Multi-orbital Kondo physics of Co in Cu hosts
Phys. Rev. B 85, 085114 (**2012**)

S. Pilati and M. Troyer
The bosonic superfluid-insulator transition in continuous space
Phys. Rev. Lett. 108, 155301 (**2012**)

S.V. Streltsov, E. Gull, A.O. Shorikov, M. Troyer, V.I. Anisimov, P. Werner
Magnetic susceptibility of Ce: an LDA+DMFT study
Phys. Rev. B 85, 195109 (**2012**)

P.N. Ma, S. Pilati, X. Dai and M. Troyer
Density functional theory for atomic Fermi gases
Nature Physics 8, 601 (**2012**).

M. Dolfi, B. Bauer, M. Troyer, Z. Ristivojevic
Multigrid Algorithms for Tensor Network States
Phys. Rev. Lett., 109, 020604 (**2012**)

Peter Anders, Philipp Werner, Matthias Troyer, Manfred Sigrist, Lode Pollet
The Cooper problem and beyond in Bose-Fermi mixtures
Phys. Rev. Lett. (in press)

M. Casula, P. Werner, L. Vaughier, F. Aryasetiawan, A. J. Millis and S. Biermann
Low-energy models for correlated materials: bandwidth renormalization from Coulombic screening
Phys. Rev. Lett. in press

Group of Joost VandeVondele
Nanoscale Simulations
Department of Materials
ETH Zurich

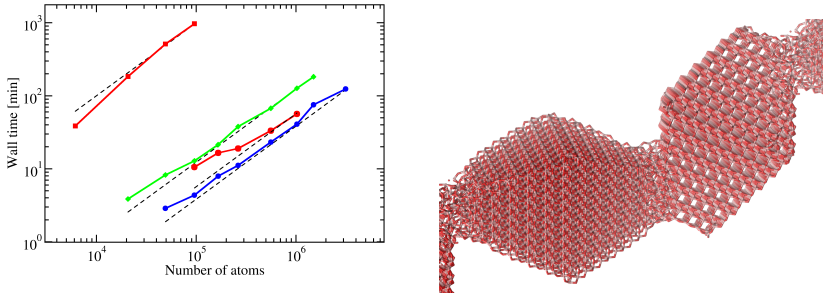
www.nanosim.mat.ethz.ch

Areas of Research:

modeling and simulation of atomistic systems, density functional theory, algorithms and high performance computing, solar cells.

Keywords:

Materials and chemistry, aqueous systems, interfaces, nanocrystals, electron transport, energy, spectroscopy, molecular dynamics, ultrafast systems, high performance computing, accelerators, algorithms, linear scaling, sparse linear algebra, CP2K.



Left panel, computational cost of large DFT calculations with CP2K now scale linearly with system size as demonstrated for condensed phase systems with full 3D periodic boundary conditions. Dashed lines represent ideal linear scaling. Right panel, model of two aggregated anatase TiO2 nanoparticles, annealed using classical molecular dynamics. Linear scaling DFT calculations allow the electronic structure of this system to be computed in 13 minutes per SCF cycle on just 75 nodes of a Cray XE6.

References

Del Ben M, Hutter J, VandeVondele J,
Second Order Møller-Plesset Perturbation Theory in the Condensed Phase: An Efficient and Massively Parallel Gaussian and Plane Waves Approach
J. Chem. Theory Comput., ASAP

VandeVondele J, Borstnik U, Hutter J,
Linear scaling self-consistent field calculations for millions of atoms in the condensed phase.
J. Chem. Theory Comput., ASAP

Cheng J, Marialore Sulpizi, VandeVondele J, Sprik M,
Hole Localization and Thermochemistry of Oxidative Dehydrogenation of Aqueous Rutile TiO2(110)
ChemCatChem, 4, 636-640 (**2012**)

VandeVondele J, Tröster P, Tavan P, Mathias G,
Vibrational spectra of phosphate ions in aqueous solution probed by first principles molecular dynamics.
J. Phys. Chem. A, 116, 2466-2474 (**2012**)

Kimmel G.A, Baer M, Petrik N.G, VandeVondele J, Rousseau R, Mundy C.J,
Polarization- and azimuth-resolved infrared spectroscopy of water on TiO2(110): Anisotropy and the hydrogen-bonding network
J. Phys. Chem. Lett., 3, 778-784 (**2012**)

Donten M.L, VandeVondele J, Hamm P,
Speed limits for acid base chemistry in aqueous solutions
Chimia, 66, 182-186 (**2012**)

Maršálek O, Uhlig F, VandeVondele J, Jungwirth P,
Structure, dynamics, and reactivity of hydrated electrons by ab initio molecular dynamics
Acc. Chem. Res., 45, 23-32 (**2012**)

Maršálek O, Elles CG, Pieniazek PA, Pluharova E, VandeVondele J, Bradforth SE, Jungwirth P,
Chasing charge localization and chemical reactivity following photoionization in liquid water.
J. Chem. Phys., 135, 224510 (**2011**)

Watkins M, Pan D, Wang EG, Michaelides A, VandeVondele J, Slater B,
Large variation in vacancy formation energies in the surface of crystalline ice.
Nat. Mater., 10, 794-798 (**2011**)

Baarman K, VandeVondele J,
A comparison of accelerators for direct energy minimization in electronic structure calculations.
J. Chem. Phys., 134(24): 244104 (**2011**)

Donten M, Hamm P, VandeVondele J,
A consistent picture of the proton release mechanism of oNBA in water by ultrafast spectroscopy and ab initio molecular dynamics.
J. Phys. Chem. B, 115(5): 1075-1083 (**2011**)

Group of Wilfred F. van Gunsteren
Computer-aided chemistry/
Informatikgestützte Chemie (igc)
ETH Zürich

www.igc.ethz.ch & www.gromos.net

Areas of Research:

1. Development of algorithms for efficient searching and sampling of configuration space
2. Simulation of long-time scale events
3. Testing and improvement of molecular models and force fields by comparison of of simulation results to experimental data
4. Simplification of force fields
5. Methods for calculating free energy and entropy differences in molecular systems
6. Representation of electrostatic interactions in molecular simulations
7. Role of electrostatic interactions in (bio-)molecular systems
8. Determination of spatial molecular structure on the basis of NMR data
9. Determination of spatial molecular structure on the basis of X-ray diffraction data
10. Quantum-mechanical simulation of biochemical phenomena
11. Development of simulation software
12. Application of simulation techniques to dynamically or functionally interesting systems or phenomena

References

Z. Lin, N. Schmid, W.F. van Gunsteren
The effect of using a polarizable solvent model upon the folding equilibrium of different β-peptides
Mol. Phys. 109 (**2011**) 493-506, DOI: 10.1080/00268976.2010.532163

A.P.E. Kunz, A.P. Eichenberger, W.F. van Gunsteren
A simple, efficient polarisable molecular model for liquid carbon tetrachloride
Mol. Phys. 109 (**2011**) 365-372, DOI: 10.1080/00268976.2010.533208

S. Riniker, W.F. van Gunsteren
A simple, efficient polarisable coarse-grained water model for molecular dynamics simulations
J. Chem. Phys. 134 (**2011**) 084110, DOI: 10.1063/1.3553378

Z. Lin, F.H. Hodel, W.F. van Gunsteren
Influence of variation of a side chain on the folding equilibrium of a β-peptide
Helv. Chim. Acta. 94 (**2011**) 597-610, DOI: 10.1002/hlca.201100003, incl. supp. mat.

B. Keller, P.H. Hünenberger, W.F. van Gunsteren
An analysis of the validity of Markov state models for emulating the dynamics of classical molecular systems and ensembles
J. Chem. Theory Comput. 7 (**2011**) 1032-1044, DOI: 10.1021/ct200069c

J.R. Allison, K. Boguslawski, F. Fraternali, W.F. van Gunsteren
A refined, efficient mean solvation force model that includes the interior volume contribution
J. Phys. Chem. B 115 (**2011**) 4547-4557, DOI: 10.1021/jp2017117, incl. supp. mat.

B. Horta, P.F.J. Fuchs, W.F. van Gunsteren, P.H. Hünenberger
New interaction parameters for oxygen compounds in the GROMOS force field: improved pure-liquid and solvation properties for alcohols, ethers, aldehydes, ketones, carboxylic acids and esters.
J. Chem. Theory Comput. 7 (**2011**) 1016-1031, DOI: 10.1021/ct1006407

A.P.E. Kunz, W.F. van Gunsteren
Enhancing the configurational sampling of ions in aqueous solution using adiabatic decoupling with translational temperature scaling
J. Phys. Chem. B 115 (**2011**) 2931-2936, DOI: 10.1021/jp110778k

D. Steiner, C. Oostenbrink, F. Diederich, M. Zürcher, W.F. van Gunsteren Calculation of binding free energies of inhibitors to Plasmepsin II
J. Comput. Chem. 32 (**2011**) 1801-1812, DOI: 10.1002/jcc.21761, incl. supp. mat.

S. Riniker, A.P.E. Kunz, W.F. van Gunsteren
On the calculation of the dielectric permittivity and relaxation time of molecular models in the liquid phase
J. Chem. Theory Comput. 7 (**2011**) 1469-1475, DOI: org/10.1021/ct100610v

W. Huang, Z. Lin, W.F. van Gunsteren
Validation of the GROMOS 54A7 force field with respect to β-peptide folding
J. Chem. Theory Comput. 7 (**2011**) 1237-1243, DOI: org/10.1021/ct100747y

Z. Lin, W.F van Gunsteren, H. Liu
Conformational state-specific free energy differences by one-step perturbation: protein secondary structure preferences of the GROMOS 43A1 and 53A6 force fields
J. Comput. Chem. 32 (**2011**) 2290-2297, DOI: 10.1002/jcc.21818, incl. supp. mat.

N. Schmid, A.P. Eichenberger, A. Choutko, S. Riniker, M. Winger, A.E. Mark, W.F. van Gunsteren
Definition and testing of the GROMOS force-field versions: 54A7 and 54B7
Eur. Biophys. J. 40 (**2011**) 843-856, DOI: 10.1007/s00249-011-0700-9, incl. supp. mat.

S. Riniker, C.D. Christ, N. Hansen, A.E. Mark, P.C. Nair, W.F. van Gunsteren
Comparison of enveloping distribution sampling and thermodynamic integration to calculate binding free energies of phenylethanolamine N-methyltransferase inhibitors
J. Chem. Phys. 135 (**2011**) 024105, DOI: 10.1063/1.3604534, incl. supp. mat.

A. Kuzmanic, D. Kruschel, W.F. van Gunsteren, B. Zagrovic
Dynamics may significantly influence the estimation of interatomic distances in biomolecular X-ray structures
J. Mol. Biol. 411 (**2011**) 286-297, DOI: 10.1016/j.jmb.2011.05.033, incl. supp. mat.

A.P.E. Kunz, H. Liu, W.F. van Gunsteren
Enhanced sampling of particular degrees of freedom in molecular systems based on adiabatic decoupling and temperature or force scaling
J. Chem. Phys. 135 (**2011**) 104106, DOI:10.1063/1.3629450, incl. supp. mat.

J. Dolenc, S. Riniker, R. Gaspari, X. Daura, W.F. van Gunsteren
Free energy calculations offer insights into the influence of receptor flexibility on ligand-receptor binding affinities
J. Computer-Aided Mol. Des. 25 (**2011**) 709-716, DOI: 10.1007/s10822-011-9453-x, incl. supp. mat.

N. Schmid, J.R. Allison, J. Dolenc, A.P. Eichenberger, A.P.E. Kunz, W.F. van Gunsteren
Biomolecular structure refinement using the GROMOS simulation software
J. Biomolecular NMR. 51 (**2011**) 265-281, DOI: 10.1007/s10858-011-9534-0

A.P.E. Kunz, W.F. van Gunsteren
A method for conformational sampling of loops in protein based on adiabatic decoupling and temperature or force scaling
ChemPhysChem 12 (**2011**) 2609-2614, DOI: 10.1002/cphc. 201100305

A.P. Eichenberger, J.R. Allison, J. Dolenc, D.P. Geerke, B.A.C. Horta, K. Meier, C. Oostenbrink, N. Schmid, D. Steiner, D. Wang, W.F. van Gunsteren
GROMOS++ software for the analysis of biomolecular simulation trajectories
J. Chem. Theory. Comp. 7 (**2011**) 3379-3390, DOI: 10.1021/ct2003622

Z. Lin, W.F. van Gunsteren
Exploring the effect of side-chain substitutions upon the secondary structure preferences of β-peptides
J. Phys. Chem. B 115 (**2011**) 12984-12992, DOI: 10.1021/jp2053508

N. Hansen, P. Kraus, H. Sassmannshausen, T. Timmerscheidt, W.F. van Gunsteren
An effective force field for molecular dynamics simulations of dimethyl sulfone
Mol. Phys. 109 (**2011**) 2593-2605, DOI: 10.1080/00268976.2011.624128

S. Riniker, C.D. Christ, H.S. Hansen, P.H. Hünenberger, C. Oostenbrink, D. Steiner, W.F. van Gunsteren
Calculation of relative free energies for ligand-protein binding, solvation and conformational transitions using the GROMOS software
J. Phys. Chem. B 115 (**2011**) 13570-13577, DOI: 10.1021/jp204303a

A. Choutko, W.F. van Gunsteren, P.H. Hünenberger
Preferential affinity of the components of liquid mixtures at a rigid non-polar surface: Enthalpic and entropic driving forces
ChemPhysChem 12 (**2011**) 3214-3223, DOI: 10.1002/cphc201100541

Z. Lin, H. Liu, S. Riniker, W.F. van Gunsteren
On the use of enveloping distribution sampling (EDS) to compute free enthalpy differences between different conformational states of molecules: application to 3_{10}-, α, and π helices
J. Chem. Theory. Comp. 7 (**2011**) 3884-3897, DOI: 10.1021/ct200623b, incl. supp. mat.

J.R. Allison, M. Bergeler, N. Hansen, W.F. van Gunsteren
Current computer modeling cannot explain why two highly similar sequences fold into different structures
Biochemistry 50 (**2011**) 10965-10973 DOI: 10.1021/bi2015663, incl. supp. mat.

D.A. Niggli, M.O. Ebert, Z. Lin, D. Seebach, W.F. van Gunsteren
Helical content of a β3-octapeptide in methanol: Molecular dynamics simulations explain a seeming discrepancy between conclusions derived from CD and NMR data
Chem. Eur. J. 18 (**2012**), 586-593, DOI: 10.1002/chem.201102667, incl. supp. mat.

A.P. Eichenberger, L.J. Smith, W.F. van Gunsteren
Ester-linked hen egg white lysozyme shows a compact fold in a molecular dynamics simulation -possible causes and sensitivity of experimentally observable quantities to structural changes maintaining this compact fold
FEBS Journal 279 (**2012**), 299-315, DOI: 10.1111/j.1742-4658.2011.08424.x, incl. supp. mat.

K. Meier, W. Thiel, W.F. van Gunsteren
On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations
J. Comput. Chem. 33 (**2012**), 363-378, DOI: 10.1002/jcc.21962

A.P.E. Kunz, J.R. Allison, D.P. Geerke, B.A.C. Horta, P.H. Hünenberger, S. Riniker, N. Schmid, W.F. van Gunsteren
New functionalities in the GROMOS biomolecular simulation software
J. Comput. Chem. 33 (**2012**), 340-353, DOI: 10.1002/jcc.21954

N. Schmid, C.D. Christ, M.Christen, A.P. Eichenberger, W.F. van Gunsteren
Architecture, implementation and parallelization of the GROMOS software for biomolecular simulation
Comp. Phys. Comm. 183 (**2012**), 890-903, DOI: 10.1016/j.cpc.2011.12.014

N. Hansen, J. Dolenc, M. Knecht, S. Riniker, W.F. van Gunsteren
Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsin-DNA duplex complexes in aqueous solution
J. Comput. Chem. 33 (**2012**) 640-651, DOI: 10.1002/jcc.22879, incl. supp. mat

J.R. Allison, S. Riniker, W.F. van Gunsteren
Coarse-grained models for the solvents dimethyl sulfoxide, chloroform and methanol
J. Chem. Phys. 136 (**2012**) 054505, DOI: 10.1063/1.3681140, incl. supp. mat.

S. Riniker, B.A.C. Horta, B. Thijssen, S. Gupta, W.F. van Gunsteren, P.H. Hünenberger
Temperature dependence of the dielectric permittivity of acetic acid, propionic acid and their methyl esters: A molecular dynamics simulation study
ChemPhysChem 13 (**2012**) 1182-1190, DOI:10.1002/cphc.201100949

A.P.E. Kunz, Z. Lin, W.F. van Gunsteren
Test of a method for sampling the internal degrees of freedom of a flexible solute molecule based on adiabatic decoupling and temperature or force scaling
Mol. Phys. 110 (**2012**) 407-417, DOI:10.1080/00268976.2011.650716

D. Steiner, C. Oostenbrink, W.F. van Gunsteren
Calculation of the relative free energy of oxidation of azurin at pH 5 and pH 9
J. Comput. Chem. 33 (**2012**) 1467-1477, DOI: 10.1002/jcc.22972, incl. supp. mat.

D. Steiner, W.F. van Gunsteren
An improved structural characterisation of reduced french bean plastocyanin based on NMR data and local-elevation molecular dynamics simulation
Eur. Biophys. J. 41 (**2012**) 579-595, DOI: 10.1007/s00249-012-0824-6, incl. supp. mat.

D. Steiner, J.R. Allison, W.F. van Gunsteren
On the calculation of 3 Jβ -coupling constants for side chains in proteins
J. Biomol. NMR 53 (**2012**) 223-246, DOI: 10.1007/s10858-012-9634-5, incl. supp. mat.

S. Riniker, W.F. van Gunsteren
Mixing coarse-grained and fine-grained water in molecular dynamics simulations of a single system
J. Chem. Phys. 137 (**2012**) 044120, DOI: 10.1063/1.4739068

S. Riniker, A.P. Eichenberger, W.F. van Gunsteren
Structural effects of an atomic-level layer of water molecules around proteins solvated in supra-molecular coarse-grained water
J. Phys. Chem. B 116 (**2012**) 8873-8879, DOI: 10.1021/jp304188z, incl. supp. mat.

Z. Lin, T.A. Timmerscheidt, W.F. van Gunsteren
Using enveloping distribution sampling (EDS) to compute the free enthalpy difference between right-and left-handed helices of a β-peptide in solution
J. Chem. Phys. 137 (**2012**) 064108, DOI: 10.1063/1.4742751, incl. supp. mat.

S. Riniker, A.P. Eichenberger, W.F. van Gunsteren
Solvating atomic level fine-grained proteins in supra-molecular level coarse-grained water for molecular dynamics simulations
Eur. Biophys. J. 41 (**2012**) 647-661, DOI: 10.1007/s00249-012-0837-1

B.A.C. Horta, Z. Lin, W. Huang, S. Riniker, W.F. van Gunsteren, P.H. Hünenberger
Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: influence on the folding properties of two beta-peptides in methanol
J. Comput. Chem. 33 (**2011**) 1907-1917, DOI: 10.1002/jcc.23021

S. Riniker, J.R. Allison, W.F. van Gunsteren
On developing coarse-grained models for biomolecular simulation: a review *Phys. Chem. Chem. Phys.* 14 (**2012**) 12423-12430, DOI:10.1039/C2CP40934H

W. Huang, A.P. Eichenberger, W.F. van Gunsteren
Molecular dynamics simulation of thionated hen egg white lysozyme
Prot. Sci. 21 (**2012**) 1153-1161, DOI:10.1002/pro.2102, incl. supp. mat.

K. Meier, N. Schmid, W.F. van Gunsteren
Interfacing the GROMOS (bio) molecular simulation software to quantum-chemical program packages
J. Comput. Chem. 33 (**2012**) 2108-2117, DOI: 10.1002/jcc.23047

D. Wang, W.F. van Gunsteren, Z. Chai
Recent advances in computational actinide chemistry
Chem. Soc. Rev. (**2012**) accepted

K. Meier, W.F. van Gunsteren
On the use of advanced modelling techniques to investigate the conformational discrepancy between two X-ray structures of the AppA BLUF domain
Phys. Chem. Chem. Phys (**2012**) submitted

A. Choutko, W.F. van Gunsteren
Exploration of swapping enzymatic function between two proteins: simulation study of Chorismate mutase and isochorismate pyruvate lyase
ChemBioChem (**2012**), submitted, incl. supp. mat.

A. Choutko, W.F. van Gunsteren
Molecular dynamics simulation of the last step of a catalytic cycle: product release from the active site of the enzyme chorismate mutase of mycobacterium tuberculosis
Prot. Sci. (**2012**) accepted, DOI: 10.1002/pro.2143, incl. supp. mat.

A. Choutko, W.F. van Gunsteren
Conformational preferences of a β-octapeptide as function of solvent and force-field parameters
Helv. Chim. Acta (**2012**) accepted, incl. supp. mat.

W.F. van Gunsteren, J. Dolenc
Thirty-five of biomolecular simulation: development of methodology, force fields, and software
Mol. Sim. (**2012**) accepted

M.M. Müller, J.R. Allison, N. Hongdilokkul, L. Gaillon, P. Kast, W.F. van Gunsteren, Ph. Marliére, D. Hilvert
Directed evolution of a model primordial enzyme provides insights into the development of the genetic code
Nat. Chem. Biol. (**2012**) submitted, incl. supp. mat.

W.F. van Gunsteren
The seven sins of academic behaviour and research in the natural sciences
Angew. Chem. (**2012**) accepted

Z. Lin, W.F. van Gunsteren
On the choice of a reference state for one-step perturbation calculations between polar and non-polar molecules in a polar environment
J. Comput. Chem. (**2012**) accepted, incl. supp. mat.

S. Riniker, L.J. Barandun, F. Diederich, O. Krämer, A. Steffen, W.F. van Gunsteren
Free enthalpies of replacing water molecules in protein binding pockets
J. Computer-Aided Mol. Des. (**2012**) submitted, incl. supp. mat.

W. Huang, S. Riniker, W.F. van Gunsteren
Rapid sampling of folding equilibria of β-peptides in methanol using a supra-molecular solvent model
J. Chem. Theory Comput. (**2012**) submitted

J.H. Missimer, M.O. Steinmetz, W.F. van Gunsteren, J. Dolenc
Influence of 63Ser phosphorylation and dephosphorylation on the structure of the stathmin helical nucleation sequence: A molecular dynamics study
Biochemistry (**2012**) accepted, incl. supp. mat.

K. Meier, A. Choutko, S. Riniker, W.F. van Gunsteren
Multi-resolution simulation in chemistry: methodological issues and exploration of the origins of differential catalysis observed between two structurally similar enzymes
Angew. Chem. (**2012**) submitted

L.J. Smith, W.F. van Gunsteren, J.R. Allison
Multiple binding modes for palmitate to barley lipid transfer protein facilitated by the presence of proline by the presence of proline 12
Prot. Sci. (**2012**) submitted, incl. supp. mat.

D. Wang, F. Freitag, Z. Gattin, H. Haberkern, B. Jaun, M. Siwko, R. Vyas, W.F. van Gunsteren, J. Dolenc
Validation of the GROMOS 54A7 force field regarding mixed α/β peptide molecules
Helv. Chim. Acta (**2012**) submitted, incl. supp. mat.

A. Eichenberger, W.F. van Gunsteren, L.J. Smith, J.Dolenc
On the effect TFE cosolvent upon the structure of hen egg-white lysozyme: a molecular dynamics simulation study based on NMR data
Biochemistry (**2012**) submitted, incl. supp. mat.

8 Acknowledgements

The C^4 Steering Committee wishes to acknowledge the excellent collaboration with the High Performance Computing Group of the ETH Informatikdienste, lead by Dr. Oliver Byrde.

We also acknowledge the ETH Department of Chemistry and Applied Biosciences (D-CHAB), and in particular its chairman, Prof. Detlef Günther, for its generous support.

Finally, we wish to thank the C^4 community for its active participation in our programs.