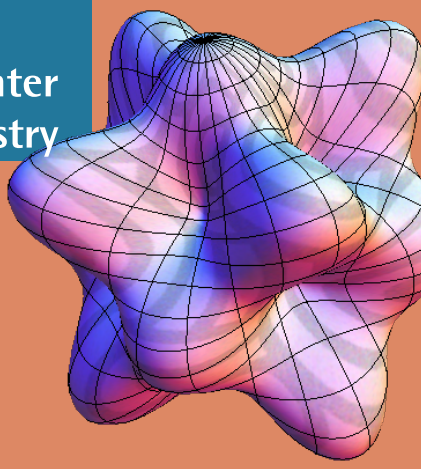
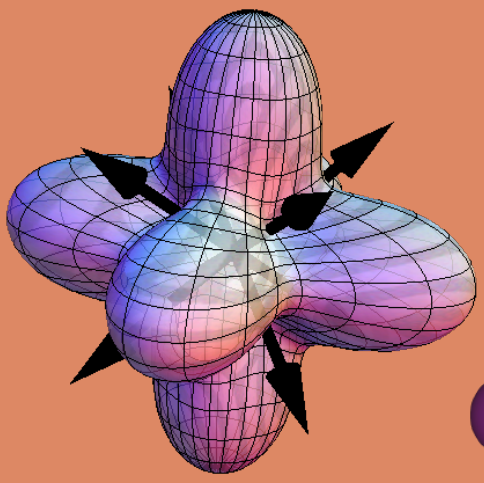
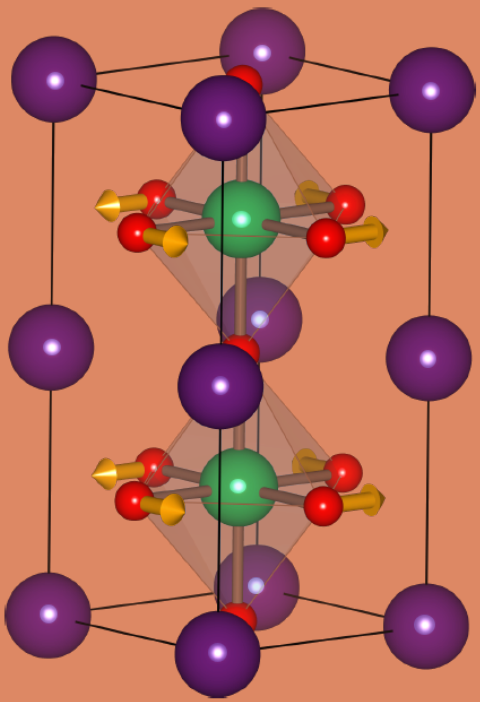
Annual Report
2012 – 2014

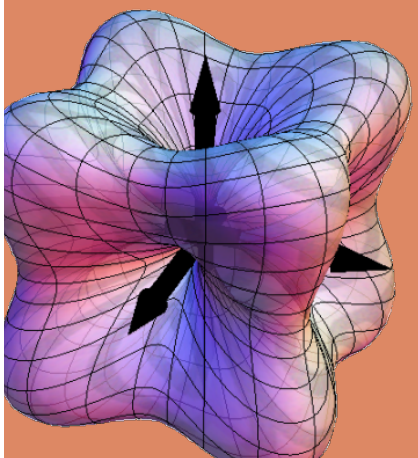
[C⁴]

Competence Center for Computational Chemistry









ETH zürich

University of Zurich[UZH]

Annual Report

[C4]

Competence Center for Computational Chemistry

July 2012 to June 2014

Impressum

Edited by:
Halua Pinto de Magalhães, ETH Zürich

Copies of this report can be downloaded from:
www.c4.ethz.ch

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Cover:
Carlo Weingart, winner of the 2013 IBM Research Forschungspreis

"Illustration of lattice instabilities in perovskites and energy surfaces for cubic single-ion anisotropies."

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 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 (till 2013), 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 20th Annual Report of the Competence Center for Computational Chemistry [C^4] reporting on its activities between July 2012 and June 2014. We also encourage you to visit our website, www.c4.ethz.ch .

2 The Past Two Years in Review

About this C4 Annual Report

Over the past two decades, the C^4 Network has grown substantially, and it became increasingly difficult to present the full scope of the research activities in the Annual Report. Therefore, in 2012 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 way, the Annual Report still gives a comprehensive overview over the activities of the computational chemistry community of the three partner institutions. This year, for the first time, we decided to publish the Annual Report on-line only. Among other, this has the advantage, that you can archive in your digital document library.

C4 Seminar

The actual "backbone" of C^4 is its Seminar Program. During the 2012 Fall- and 2013 Spring-Term the C^4 Seminar Program covered 11 lectures. One C^4 seminar was hosted by the IBM Research Laboratory, another three seminars were hosted by the University of Zürich.

During the 2013 Fall- and 2014 Spring-Term 10 lectures, again some of them featuring leaders in the field of computational chemistry, were presented. The seminar enjoys a remarkable popularity bringing together between forty and sixty students and researchers each time. During this academic year, one C^4 seminar was hosted by the IBM Research Laboratory, and another two seminars were hosted by the University of Zürich. One of the seminars, presented by Prof. Keiji Morokuma (Kobe and Emory Universities), was part of a Swiss Chemical Society Lectureship.

Compute Resource

Since many of the members of the computational chemistry community have their own computing facilities, or were granted compute time by the Centro Svizzero die Calcolo Scientifico (CSCS), the compute resource offered by C^4 in recent years became less and less "mission critical". C^4 holds a number of nodes on the ETH Brutus cluster that are open to all ETH computational chemists.

The IBM Research Award

The "IBM Research Forschungspreis" is a prize for outstanding MSc and PhD theses in the area of computer-modelling and simulation in chemistry, biology and materials science sponsored by the IBM Zürich Research Laboratory. The Forschungspreis was awarded first time in 2007.

In 2012, the prize was awarded to Konrad Marti of the group of Prof. Markus Reiher for his PhD thesis entitled "New Electron Correlation Theories and Haptic Exploration of Molecular Systems". The award jury consisted of Professors U.W. Suter (chairperson and former VP Research ETH Zürich), Jürg Hutter (UZH) and Alessandro Curioni (IBM Research).

In 2013, the prize was awarded to Carlo Weingart of the group of Prof. Nicola Spaldin (ETH D-MATL) for his MSc thesis entitled "Origin of Spin Canting in Multiferroic Perovskites". The award jury consisted of Professors U.W. Suter (chairperson), Hans P. Lüthi (ETH), Jürg Hutter (UZH) and Alessandro Curioni (IBM Research).

The 2012 and 2013 Award Ceremonies both took place at the ETH Tag, with the Rector, Prof. Lino Guzzella, handing out the award to the two winners. The laureates, Carlo Weingart, now computational scientist at Autoform Development GmbH in Zürich, and Konrad Marti, now consultant at Credit Suisse, also presented their research at the occasion of two special C^4 Seminars held at the IBM Research Laboratory in Rüschlikon (see C^4 Programs).

New Members of the C4 Community, Retirements from professorship (Emeritierungen), and Colleagues Leaving

During the reporting period, two of the C4 protagonists retired from professorship: Prof. Wilfred van Gunsteren and Prof. Martin Quack both gave their farewell lectures in 2013 and 2014, respectively. The recordings of both lectures can be viewed on the ETH Zürich Multimedia Portal. Wilfred van Gunsteren and Martin Quack both continue their research at ETH Zurich with support from their respective ERC Advanced Grants.

Profs. Kim Baldridge, Ive Hermans, and Franziska Schoenebeck accepted faculty positions at Tianjin University, UW Madison, and the RWTH in Aachen.

Sereina Riniker, former Presidential Fellow the Novartis Institutes for Biomedical Research, was appointed assistant professor at ETH Zürich. Sereina also won an IBM Research Forschungspreis for her MSc thesis in 2009.

Outlook

A network such as C^4 plays an important role when it comes to the exchange of information within a relatively large and distributed community. Modeling and Simulation have become established tools also for researchers with an experimental background, and the C^4 network gives them access to the state-of-the-art methodologies and computational know-how. Also in the next year we will make sure that C^4 is a valuable platform for its stakeholders.

Hans P. Lüthi, Leiter C^4
December, 2014

3 The C4 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. The University of Zürich is represented by its newly established Department of Chemistry, and the IBM Research Laboratory by its Computational Science Division.

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 C4 community

Research Group	*Institute*
Prof. P. Chen*	Organic Chemistry ETH
Prof. C. Copéret	Inorganic Chemistry ETH
Prof. A. Curioni	IBM Zürich Research Laboratory
Prof. P. Hünenberger	Physical Chemistry ETH
Prof. J. Hutter	Department of Chemistry UNI ZH
PD Dr. H.P. Lüthi	Physical Chemistry ETH

Research Group	*Institute*
Prof. M. Parrinello	Physical Chemistry ETH
Prof. M. Quack	Physical Chemistry ETH
Prof. M. Reiher	Physical Chemistry ETH
Prof. S. Riniker**	Physical Chemistry ETH
Prof. G. Schneider	Pharmaceutical Sciences ETH
Prof. N. Spaldin*	Materials Theory ETH
Prof. M. Troyer	Theoretical Physics ETH

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

4 C4 Activities in 2012-2014

C4 Seminar

During the Fall- and Spring-Terms in the academic years from 2012 to 2014 the C4 Seminar Program covered 21 lectures, again some of them presented by leaders in the field of computational chemistry. Two C4 seminars were hosted by the University of Zurich.

C4 Tutorials

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

C4 Workshop

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

On the next four 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 2012

Auditorium HCI J6, ETH Hönggerberg
13:00-14:00 (unless otherwise noticed)

16. 10. 2012 (*hosted by ETH Zürich Kolloquium für Physikalische Chemie*)
Prof. Christoph van Wüllen TU Kaiserslautern (Deutschland)
Zero field splitting of multinuclear transition metal complexes: a challenge for density functional methods

01. 11. 2012 (*seminar starts at 12:00 in auditorium HCI J6*)
Dr. Lorna Smith, University of Oxford, Oxford (UK)
Ligand binding and protein misfolding: new insights from MD simulations.

08.11. 2012
Prof. Thomas F. Miller III, California Institute of Technology, Pasadena (CA, USA)
Title open

22. 11. 2012 (*hosted by University of Zürich Institute of Physical Chemistry Seminar*)
Prof. Alessandro Laio, Intl. School for Advanced Studies, SISSA, Trieste (Italy)
Exploring the universe of protein structures by atomistic simulations: beyond the Protein Data Bank

03.12. 2012
Dr. Setphane Redon, INRIA Grenoble Rhône-Alpes, Saint Ismier (France)
Theory and algorithms for adaptive particle simulations

08. 12. 2012 (*hosted by University of Zürich Institute of Physical Chemistry Seminar*)
Dr. Damien Laage, École Normale Supérieure, Paris (France)
Towards a microscopic picture of protein hydration dynamics

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 2013

Auditorium HCI J7, ETH Hönggerberg

13:00-14:00

21. 02. 2013
Dr. O. Anatole von Lilienfeld, Argonne National Laboratory**,** Argonne, IL (USA)
The Quantum Machine: Supervised learning of Schrödinger's equation in chemical compound space
(gemeinsam mit Seminar des Instituts für Physikalische Chemie, Uni Zürich)

28. 02. 2013
Prof. Jenny Nelson, Imperial College London, London (U.K.)
Organic solar cells: from material design to system efficiency

09. 04. 2013
Prof. Martin Kaupp, TU Berlin (Deutschland)
Computational Magnetic Resonance Spectroscopy: Challenges and Applications of Quantum-Chemical Methods
(gemeinsam mit Kolloquium für Physikalische Chemie, ETH Zürich)

11. 04. 2013
Dr. Volker Blum, Fritz-Haber-Institut, Berlin (Deutschland)
An Integrated All-Electron Framework for Materials, Molecules and the Chemistry that They Control: FHI-aims

18. 04. 2013
2012 IBM Research Forschungspreis Award Lecture
Dr. Konrad Marti, Credit Suisse, Zürich (Schweiz)
New Electron Correlation Theories and Haptic Exploration of Molecular Systems
(findet im IBM Forschugslaboratorium in Rüschlikon statt)

02. 06. bis 07.06.2013
7th Molecular Quantum Mechanics Congress (MQM2013)
Palazzo dei Congressi / USI Lugano, Lugano (Schweiz)

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 Herbstsemester 2013

Auditorium HCI J3, ETH Hönggerberg

13:00-14:00 (for lectures at ETH only)

01. 10. 2013 (*hosted by University of Zürich Department of Chemistry Seminar**)
Prof. Dr. Frank Neese, MPI for Chemical Energy Conversion, Mülheim/Ruhr (D)
Insights into the Chemistry of Biological Energy Conversion from a Combination of Spectroscopy and Quantum Chemistry

10. 10. 2013 (*hosted by University of Zürich Institute of Physical Chemistry Seminar***)
Prof. Dr. Ernst-Walter Knapp, Freie Universität Berlin, Berlin (D)
Marriage of Quantum Chemistry and Electrostatics to Compute Accurate pKa's and Redox Potentials in Solution and for Proteins

14.11. 2013 *(with ETH Zürich Kolloquium für Physikalische Chemie)*
Prof. Dr. Alexandre Bonvin, Utrecht University, Utrecht (NL)
Modelling Structure, Affinity and Specificity of Biomolecular Complexes

28. 11. 2013
Prof. Dr. Karsten Reuter, Technische Universität München, Garching (D)
From Electrons to the Reactor: Multiscale Modeling of Catalytic Processes

05.12. 2013
Prof. Dr. Francesco Evangelista, Emory University, Atlanta, Georgia (USA)
Multireference Coupled Cluster Theory: Breakthroughs and Challenges

*) Auditorium Y15-G-19 at 17:00
**) Seminarraum 34-K-01 at 10:15

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 2014

Auditorium HCI J7, ETH Hönggerberg

13:00-14:00

27. 02. 2014
Prof. Sabre Kais, Perdue University**,** West Lafayette, Indiana (USA), and
Qatar Environment and Energy Research Institute (QEERI), Doha (Qatar)
Light Matter Interaction: The Role of Quantum Coherence and Entanglement

20. 03. 2014
Prof. Nicola Marzari, EPF Lausanne, Lausanne (Switzerland)
The Density is not Enough

10. 04. 2014
IBM Research Forschungspreis Award Lecture
Carlo Weingart, MSc.,
AutoForm Development GmbH, Zürich (Switzerland)
From Computational Materials Science to Virtual Sheet Metal Forming
(findet am IBM Forschungslaboratorium in Rüschlikon statt)

08. 05. 2014
Prof. Sam de Visser, University of Manchester, Manchester (UK)
Computational Studies into the Origin of the Reactivity and Catalytic Properties of Iron-containing Wild-type and Bioengineered Enzymes

22. 05. 2014
Swiss Chemical Society Lectureship
Prof. Keiji Morokuma, Kyoto University, Kyoto (Japan), and
Emory University, Atlanta, Georgia (USA)
Title to be announced

www.c4.ethz.ch

5 IBM Research Forschungspreis

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 2014 IBM Research Forschungspreis was issued at the end of the Spring Term. It is for PhD theses submitted during the past two years.

The Winner of the 2013 IBM Research Prize:

Carlo Weingart (Group of Prof. N. Spaldin)

Department of Materials ETH Zürich

The Award Jury, consisting of Profs. A. Curioni, U.W. Suter and PD Dr. H.P. Lüthi awarded Carlo Weingart the IBM Research Forschungspreis for his innovative MSc thesis entitled "Origin of spin canting in multiferroic perovskite". In their laudatio, the Award Jury states that

"Herr Weingart hat sich dem Problem gewidmet, was die Ursache der schlecht verstandenen Kopplung zwischen anti-ferromagnetischem und ferroelektrischem Verhalten gewisser Materialien sei. Die Frage ist sowohl von theoretischer Bedeutung als auch wichtig für die praktische Entwicklung von Materialien, bei denen Magnetisierung und elektrische Polarisation gekoppelt sein sollen. Durch geschickte Anwendung von Dichte-Funktional-Methoden zur Berechnung der elektronischen Struktur von Kristallen und der aus der Symmetrie-Theorie stammenden Zwangsbedingungen für Elemente der berechneten Eigenschaften gelang es ihm, unerwartete und neue Erkenntnisse zu erhalten, welche von Bedeutung für die Materialwissenschaften sein werden."

PD Dr. Hans P. Lüthi, Prof. Alessandro Curioni, Carlo Weingart and Prof. Nicola Spaldin at the Award Lecture 2014 at IBM Research Rüschlikon

Carlo Weingart, MSc Thesis 2013

"Origin of spin canting in multiferroic perovskite"

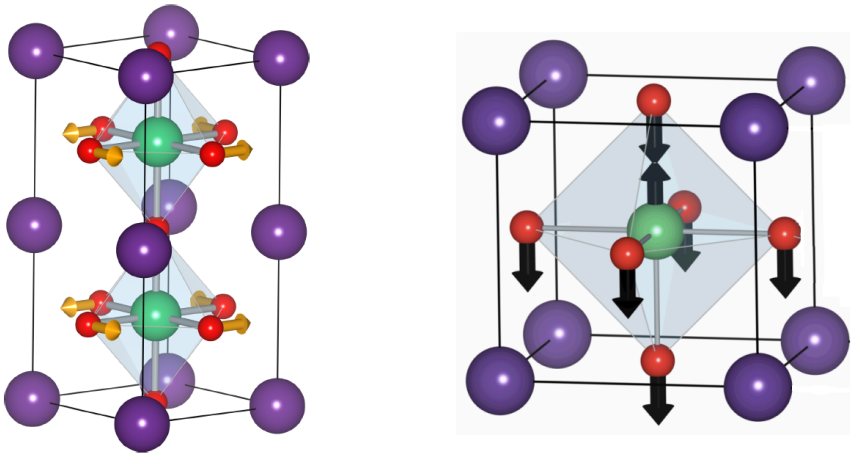


Illustration of lattice instabilities in perovskites.
(a) antiferrodistortive distortion and (b) ferroelectric distortion.
The arrows show the displacements of the atoms.

The aim of the present study is to quantify from first-principles calculations the mechanisms leading to the weak ferromagnetism ordering in two representative perovskites, $LaFeO_3$ and $BiFeO_3$. Both compounds show antiferrodistortive distortions (of different types), and $BiFeO_3$ also has a ferroelectric instability, whereas $LaFeO_3$ does not. To understand the links between these lattice distortions and the magnetism, we decompose the three main magnetic interactions, i.e. exchange, Dzyaloshinski-Moriya and single ion anisotropy, and look at how these three interactions are affected by the amplitude and the combination of the different lattice distortions. This systematic analysis allows us to understand the coupling between structural distortions and spin canting, and propose some guidelines for the design of magnetoelectric weak ferromagnetisms.

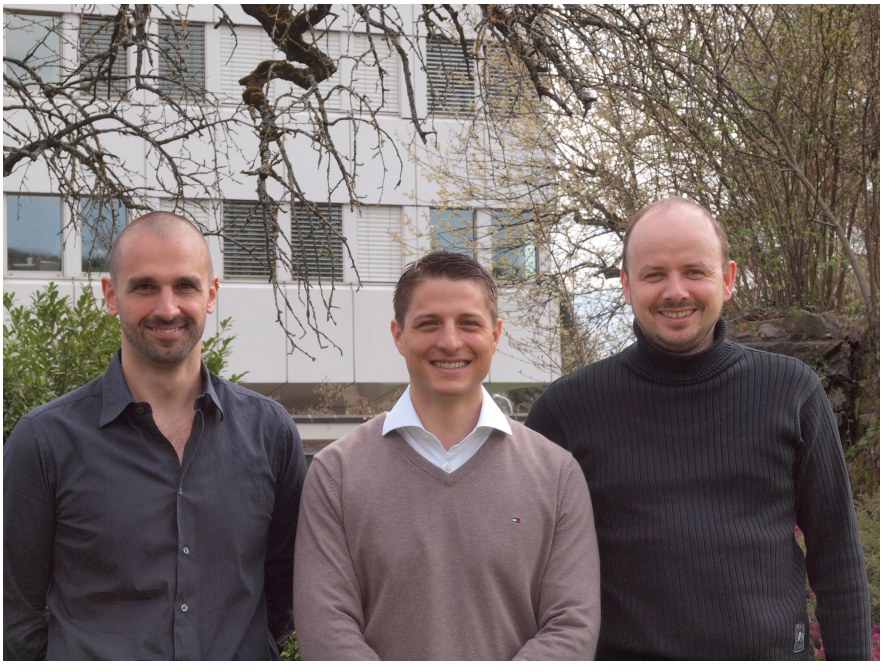
The Winner of the 2012 IBM Research Prize

Konrad H. Marti, (Group of Prof. M. Reiher)

Department of Chemistry and Applied Biosciences ETH Zürich

The Award Jury, consisting of Profs. A. Curioni, U.W. Suter and PD Dr. H.P. Lüthi awarded Konrad Marti the IBM Research Forschungspreis for his innovative PhD thesis entitled "New Electron Correlation Theories and Haptic Exploration of Molecular Systems". In their laudatio, the Award Jury states that

"Dr. Konrad H. Marti was awarded the IBM Research Prize 2012 for the development and implementation of novel wave-function parameterizations and potential-energy exploration methods as new conceptual tools for the study of molecules and their reactivity. He established truly new methods for the solution of the electronic Schrödinger equation as well as novel approaches to the assessment of potential energy surfaces; in both ways he has contributed significantly to the field of Computational Chemistry."

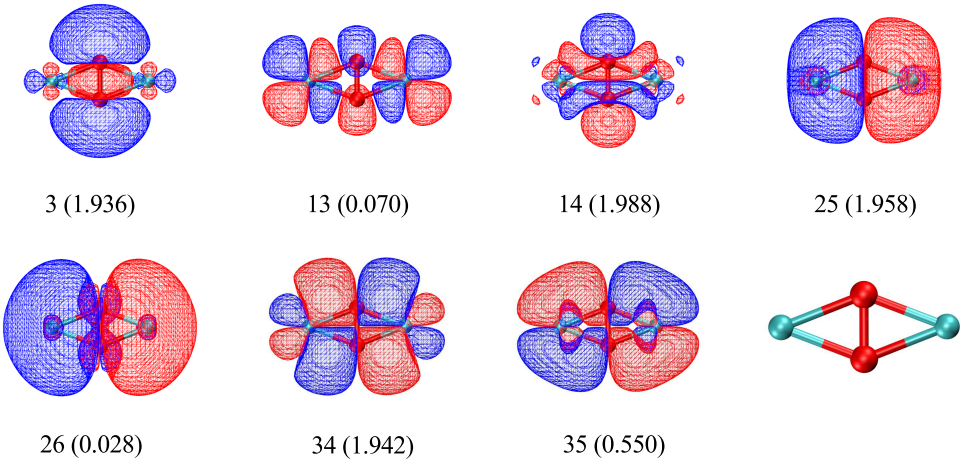


Dr. Teodoro Laino, Dr. Konrad Marti and Prof. Markus Reiher at the Award Lecture 2013 at IBM Research Rüschlikon

Konrad H. Marti, PhD Thesis 2012

"New Electron Correlation Theories and Haptic Exploration of Molecular Systems"

In transition metal catalysis, the precise characterization of the relative energies is of paramount importance. In particular, it is still a challenging task to predict energy differences between states of different spin accurately using a wide variety of modern standard quantum chemical methods. The encouraging results of the density matrix renormalization group (DMRG) algorithm for complicated molecular electronic structure theory stimulated our research in this direction. We describe how the concept of quantum information entropy can efficiently be exploited and cast into an algorithm which aims to improve the convergence of the DMRG optimization. The new code is employed to describe spin splitting in methylene and ozone, as well as the high-spin ground state of a transition metal compound.



Molecular orbital pictures of the highly entangled orbitals for the peroxo $[Cu_2O_2]^{2+}$ isomer. The number below each orbital corresponds to the orbital index and the occupation number is written in the parentheses.

Finally, we present a new way of analyzing potential energy surfaces of chemical reaction mechanisms by means of a haptic exploration. The haptic methodology is shown to allow chemists to physically experience the quantum mechanical forces acting on reactants, to actively influence the chemical reaction, and to probe different reaction channels. The haptic machinery is demonstrated at the example of the protonation of a water molecule.

Former Awardees

2011 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?"

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

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"

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"

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

6 Operation of the C4 Compute Resources

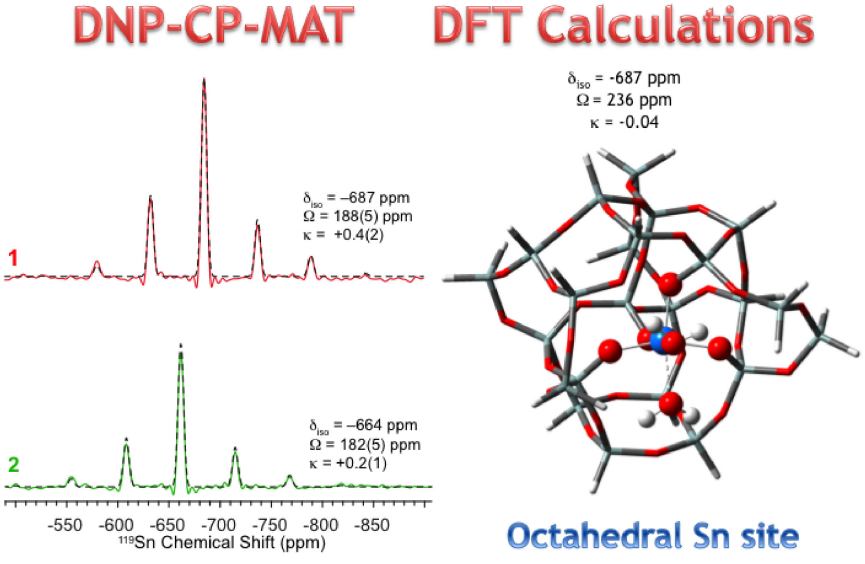
Brutus Share: Based on an infrastructure proposal supported by the Department of Chemistry and Applied Biosciences (D-CHAB), the VP Research granted an extension of the active share on Brutus by another ten standard- and five fat-nodes. The fifteen nodes with 48 cores each (12 core AMD 6174 CPUs; 4CPUs per node). The 720 core share went into production in November 2011. A renewal or extension of the share is under consdideration.

7 Research Group Portraits & Publications in 2012-2014

Overview

Group of Prof. Christophe Copéret and
Dr. A. Comas-Vives (SNF Ambizione)
Laboratory of Inorganic Chemistry
ETH Zurich

www.coperetgroup.ethz.ch



NMR Characterization of the active site of the Sn-beta zeolite.

Areas of Research:

Computational Chemistry, Surface Chemistry, Heterogeneous Catalysis

Keywords:

DFT Calculations, NMR, Reaction Mechanisms, Molecular Dynamics

References

Alphazan et al.
Highly Active Nonpromoted Hydrotreating Catalysts through the Controlled Growth of a Supported Hexagonal WS_2 Phase,
ACS Catalysis, 4, 4320-4331, (**2014**).

Wischert et al.,
Visibility of Al Surface Sites of γ-Alumina: A Combined Computational and Experimental Point of View
J. Phys. Chem. C, 118, 15292-15299, (**2014**).

Wolf, P et al.,
NMR Signatures of the Active Sites in Sn-β Zeolite
Angew. Chem. Int. Ed., 53, 10179-10183, (**2014**).

Delley et al.,
Proton transfers are key elementary steps in ethylene polymerization on isolated chromium(III) silicates
PNAS, 111, 11624-11629, (**2014**).

Conley et al.
Silica-surface reorganization during organotin grafting evidenced by 119Sn DNP SENS: a tandem reaction of gem-silanols and strained siloxane bridges,
Phys. Chem. Chem. Phys., 16, 17822-17827, 2014

Kalhor et al.,
Reactivity of silica supported zirconium hydride towards N_2O and CO_2 probe molecules: a computational point of view
New. J. Chem., 38, 3717-3721, (**2014**).

Girleanu et al.,
Magnifying the Morphology Change Induced by a Nickel Promoter in Tungsten(IV) Sulfide Industrial Hydrocracking Catalyst: A HAADF-STEM and DFT Study
ChemCatChem, 6, 1594-1598, (**2014**).

Kermagoret et al.,
Chlorodiethylaluminum supported on silica: a dinuclear aluminum surface species with bridging μ^2-Cl-ligand as a highly efficient co-catalyst for the Ni-catalyzed dimerization of ethene."
J. Catal., 313, 46-54, (**2014**).

Lapadula et al.,
Near-IR Two Photon Microscopy Imaging of Silica Nanoparticles Functionalized with Isolated Sensitized Yb(III) Centers
Chem. Mater., 26, 1062-1073, (**2014**).

Filonenko, et. al.
The impact of Metal–Ligand Cooperation in Hydrogenation of Carbon Dioxide Catalyzed by Ruthenium PNP Pincer
ACS Catal., 3, 2522-2526, (**2013**).

Vilé, et. al.,
Silver Nanoparticles for Olefin Production: New Insights into the Mechanistic Description of Propyne Hydrogenation
ChemCatChem, 5, 3750-3759, (**2013**).

Kermagoret, et. al.
Triisobutylaluminum: bulkier and yet more reactive towards silica surfaces than triethyl or trimethylaluminum
Dalton Trans., 42, 12681-12687, (**2013**).

Grau, E. et. al.
Tetrahydrofuran in $TiCl_4$/THF/$MgCl_2$: a Non-Innocent Ligand for Supported Ziegler–Natta Polymerization Catalysts
ACS Catal., 3, 52-56, (**2013**).

Group of Alessandro Curioni
Computational Sciences
IBM Zurich Research Laboratory

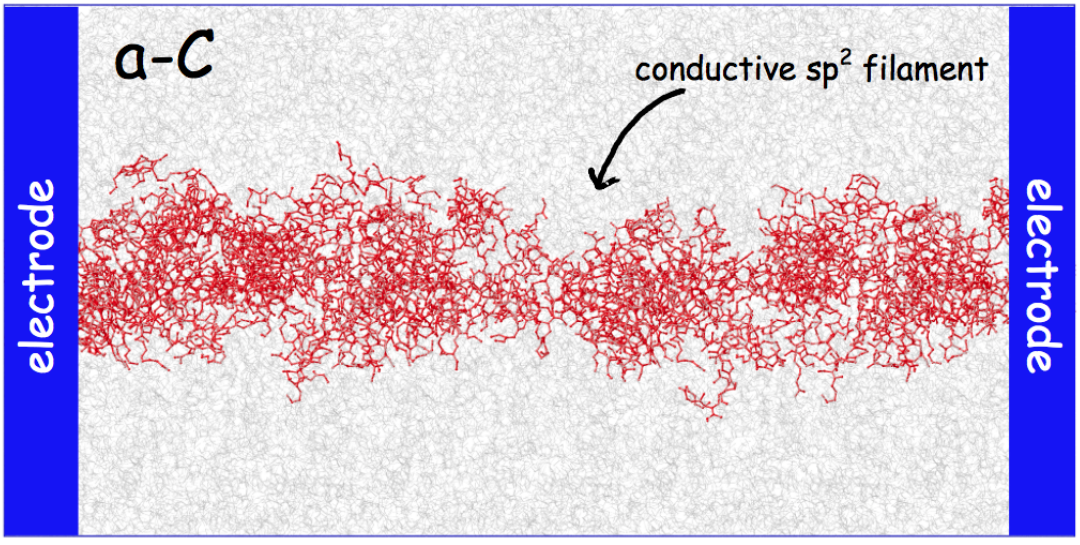
http://www.research.ibm.com/labs/zurich/cccs/

Areas of Research:

Computational Materials Science, Computational Engineering, Computational System Biology, Massively Parallel Computing

Keywords:

Materials Science, Energy Storage, Quantum Chemistry, Molecular Dynamics, Density Functional Theory, Computational Sciences, Software development, CPMD, Data Analysis



Representation of a next-generation non-volatile memory based on thin films of (sp3-rich) amorphous carbon (a-C) and conductive sp2 filaments. Information is stored via formation and destruction of the conductive sp2 filaments in a-C (CareRAMM, EU)

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Interface dipoles of organic molecules on Ag(111) in hybrid density-functional theory,
New J. Phys. 15, 083009 (**2013**)

B. Schuler, W. Liu, A. Tkatchenko, N. Moll, G. Meyer, A. Mistry, D. Fox, and L. Gross,
Adsorption geometry determination of single molecules by atomic force microscopy,
Phys. Rev. Lett. 111, 106103 (**2013**)

B. Schuler, F. Mohn, N. Moll, L. Gross, and G. Meyer,
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Physik in Unserer Zeit 44, 6 (**2013**)

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New Journal of Physics 15 (8), 083009 (**2013**)

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Visualization of Chemical Bonds,
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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

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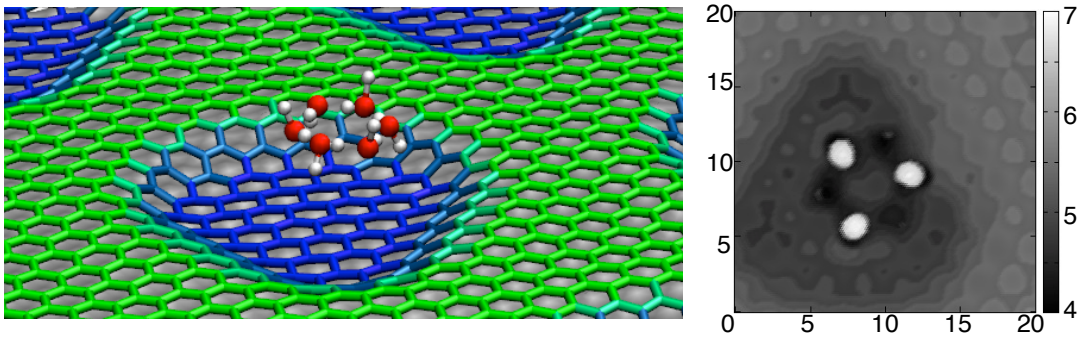
Areas of Research:

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

Keywords:

Electronic structure theory, correlation methods, large scale computing, molelcular dynamics, density functional theory, condesned phase, interfaces, liquids, solutions, chemical reactions



Water cluster adsorbed in the pore of the h-BN/Rh(111) nanomesh. The dipoles of the water molecules arrange in a homodrome hexamer and the simulated STM image, as obtained within the Tersoff-Hamann approximation, (right panel) is consistent with experimental observation.

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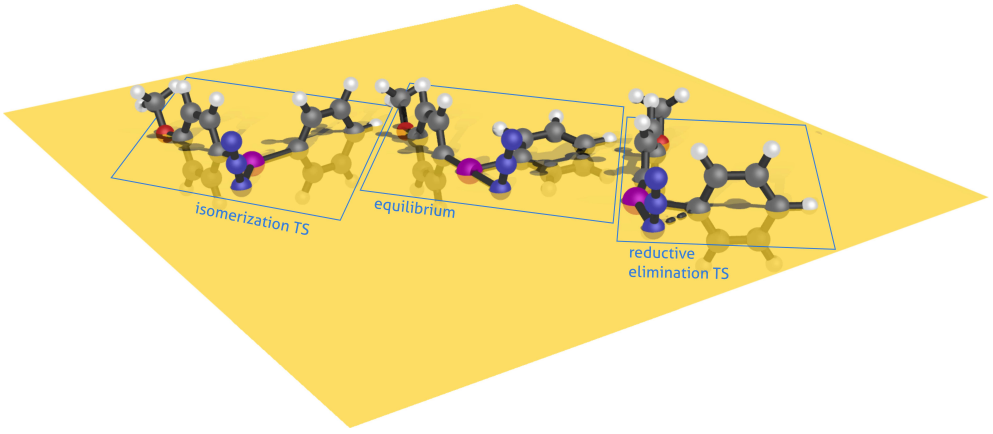

Illustration of the planarity retention of the hypervalent region of λ^3-iodanes in the course of the reductive elimination reaction.

Areas of Research:

Electronic Structure Theory and Applications, Computational Science

- Electronic structure and properties of π-conjugated compounds:Electron delocalization and the effect of donor/accptor functionalization
- Understanding 4-electron-3-center-bonds in hypervalent λ^3-iodane reagents and optimization of the reactivity
- Scientific Computing: Generation, archival, and processing of quantum chemical data at large scale to find quantitative relationships between the electronic structure and properties

Keywords:

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

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S. Ramsaywack, S. Karaca, M. Gholami, R. McDonald, F. Hampel,
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Theory, Synthesis, and Properties,
J. Org. Chem., 79, 10013-10029 (**2014**).

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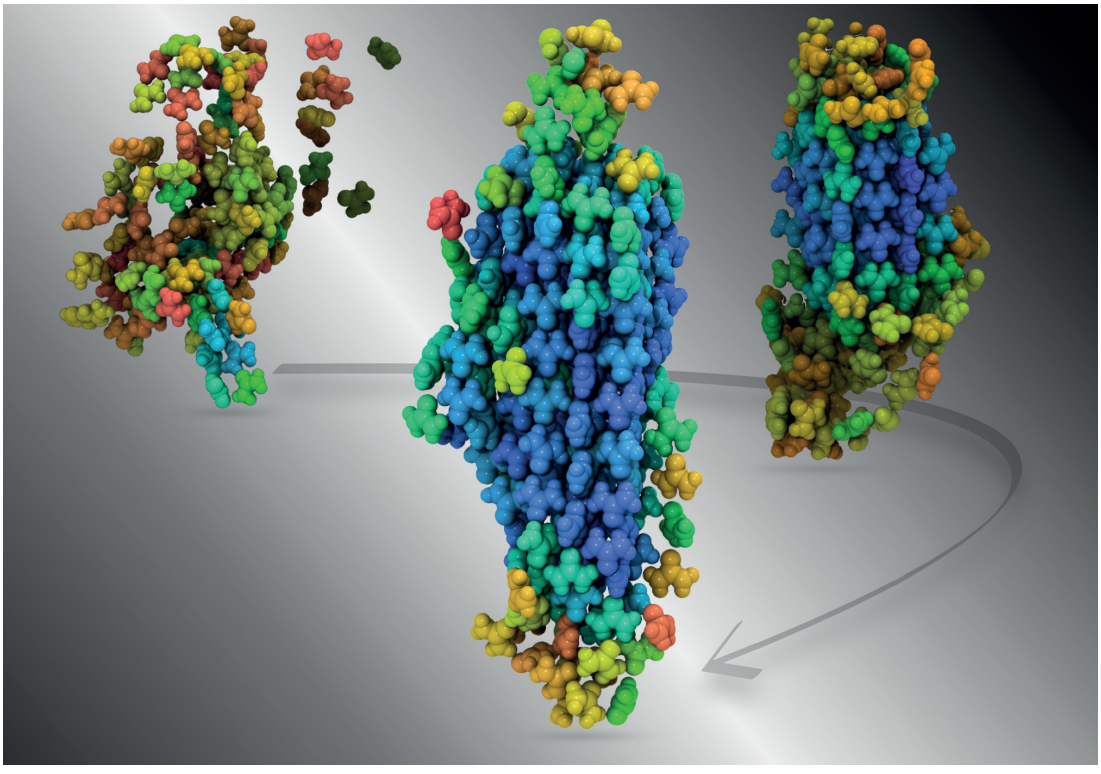
Areas of Research:

Molecular Dynamics Simulation: classical and ab-initio. Computational Science

Keywords:

Enhanced sampling; metadynamics; rare events; allostery; conformational changes in protein; protein-ligand unbinding; crystal structure nucleation; crystal growth; water



Crystal nucleation in solution: from disordered clusters to crystals
(Picture by Matteo Salvalaglio)

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Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the Fly Transition Barier Estimation
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DOI: 10.1073/pnas.1421192111

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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.

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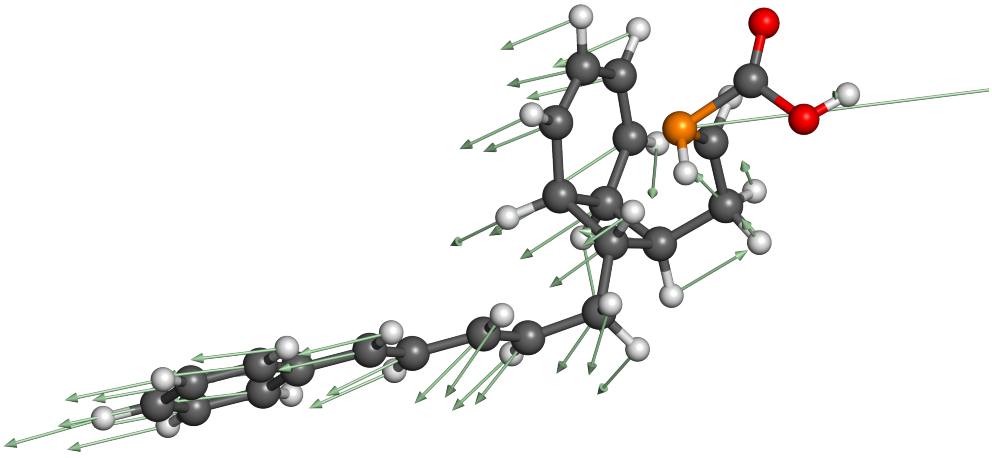

Representation of a molecular structure along with atomic forces experienced by the operator through a haptic device.[1]

Synopsis:

The main focus of the Reiher group is on the development of theory and algorithms for the calculation of electronic structures based on the first principles of quantum mechanics. The aim of our efforts is to derive quantitative means as well as concepts for understanding chemical processes. One intellectual driving force for our work is the desire to selectively extract relevant (often local) information from a strongly interacting system of particles without introducing arbitrary assumptions on the subsystem.

Areas of Research:

Relativistic Quantum Chemistry and Atomic Physics, Electron-Electron Interaction: Density Matrix Renormalization Group (DMRG), Tensor-Network States (TNS) and Density Functional Theory (DFT); Theoretical Bio-Inorganic Chemistry and Coordination Chemistry, Quantum Chemical Analysis of Novel Compounds, Vibrational Spectroscopy of Large Molecules, Haptic Quantum Chemistry

[1] M. Haag, *Theory of Chemical Reactivity in Virtual Environments,* Dissertation ETH Zurich No. 21945 (**2014**)

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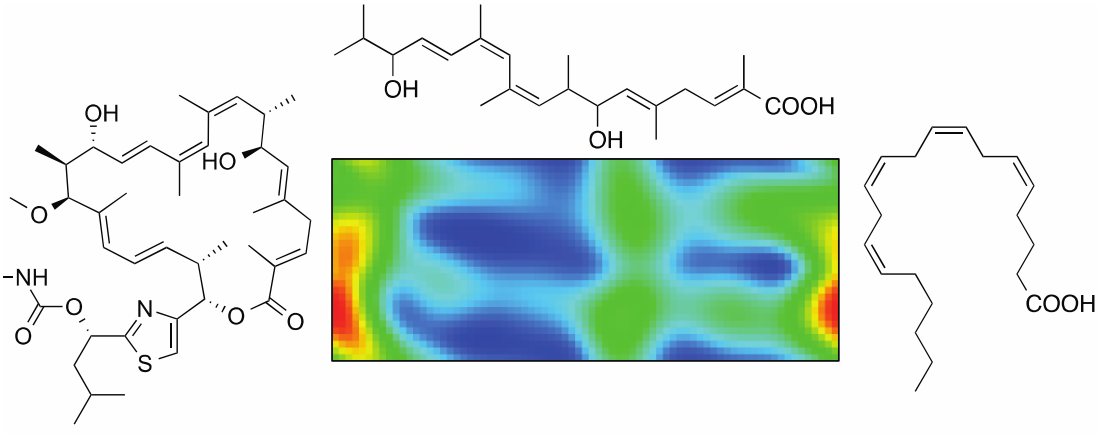
Areas of Research:

Computer-assisted Drug Design, Machine-learning, Peptide-Membrane Interaction

Keywords:

Adaptive systems, chemical similarity, de novo design, drug discovery, ligand-receptor interaction, neural networks, structure-activity relationships, target prediction



The Molecular Design Laboratory develops and implements new concepts, algorithms and software for rapid identification of bioactive tool compounds and pharmaceutical lead structures.

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Areas of Research:

Quantum many body physics, quantum computing, high performance computing, computational reproducibility ecosystems simulations

Keywords:

Computational physics, strongly correlated fermions, quantum gases, Bose Einstein condensation, quantum devices, quantum Monte Carlo, tensor network algorithms, quantum algorithms, quantum simulations, quantum many body systems, computational provenance, ecosystems simulations, remote sensing

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