PADERBORN UNIVERSITY

Paderborn Center for Parallel Computing

PROJECTS
FACTS
RESEARCH
HPC
TEACHING
PEOPLE

ANNUAL REPORT 2014/15/16

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Paderborn Center for Parallel Computing

PREFACE

PREFACE

In October 2015, I was appointed as professor at the department of Computer Science of Paderborn University. With this appointment, I have also accepted the position as the director of the Paderborn Center for Parallel Computing (PC²). This position had been vacant since 2011 and has been filled ad interim by the chairman of the board Professor Holger Karl. As I have been involved in the activities of PC² for a long time as a research collaborator and board member, I have gladly accepted the opportunity to shape the future development of the high-performance computing (HPC) services offered by PC² and to strengthen our institute's research profile through my expertise in computer systems research.

It is thus my great pleasure to present you the latest research and service report of PC². The format and contents of the report have been redesigned from the ground up. Our mission was to present you the exciting research that is enabled by our high-performance computing systems and services in a fresh and easily accessible way. The report also offers you the opportunity to look behind the scenes and learn more about our computing infrastructure, our innovative computing systems research, and the motivated team that makes almost anything possible.

Looking to the future, we can assure you that PC² will continue on the path to exciting new ventures. During the reporting period, we have prepared and submitted a proposal to the German Council for Science and Humanities (Wissenschaftsrat) for funding the project Noctua. This project comprises the installation of a new, larger scale HPC system and the construction of a future-oriented computing center building with a total budget of 25.4 million €. We are happy to report that funding for this project has been approved in June 2017. Noctua will strengthen the strategically important area of computational sciences and computing systems research at Paderborn University, allowing our researchers to continue top-level research that is nationally and internationally recognized. We are looking forward to informing you about the execution of this Noctua project in the next report.

Prof. Dr. Christian Plessl
Managing director and chairman of the board

DEVELOPMENT OF PC² IN THE REPORTING PERIOD

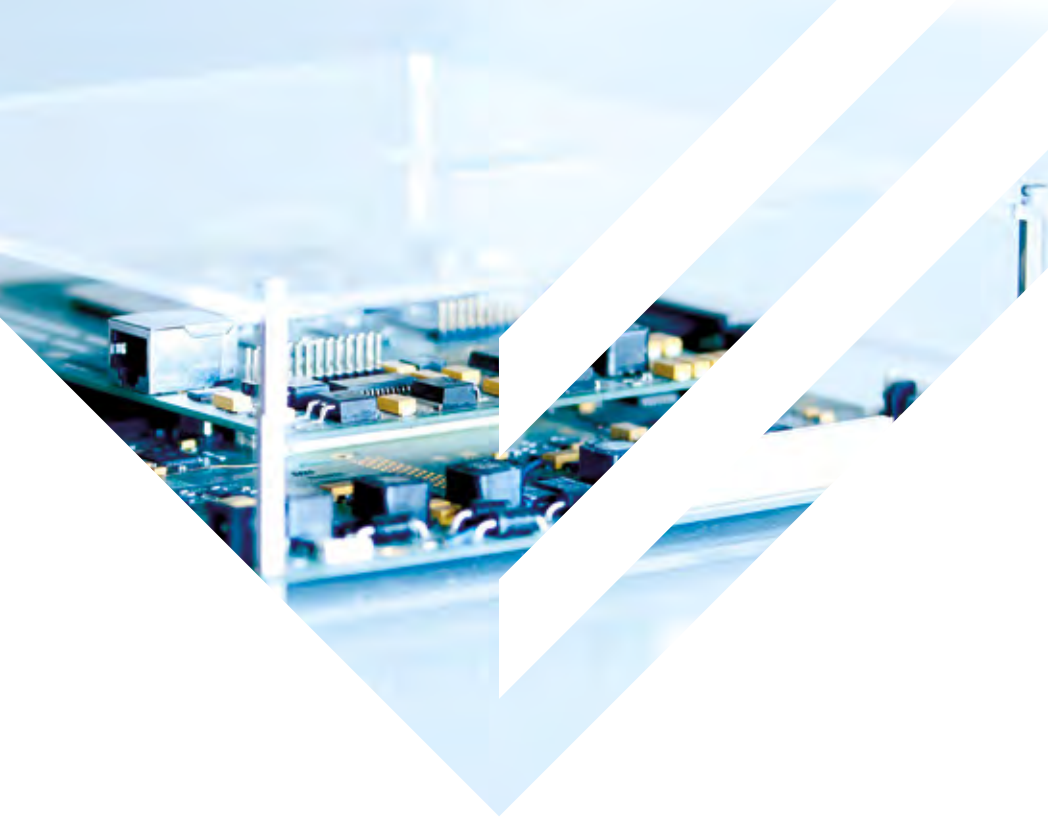
The Paderborn Center for Parallel Computing (PC²) is a scientific institute of Paderborn University. Our mission is to advance interdisciplinary research in parallel and distributed computing with innovative computer systems. We operate several high-performance cluster systems with more than 10,000 cores to provide researchers from Paderborn University and other academic institutions in North Rhine-Westfalia with HPC services. In addition, we conduct research in HPC technologies and applications in collaboration with scientists from our university and those from other national and transnational projects.

Currently, our activities are focused on three main areas:

We conduct **computing systems research** for energy-efficient HPC with an emphasis on heterogeneous and accelerated computing with Field-Programmable Gate Arrays (FPGAs) and Manycore architectures.

We collaborate with researchers from computational science to develop, optimize and benchmark **new methods for scientific simulations**, with many of these results contributing to widely-used open source codes.

We provision **HPC infrastructure and services** for computational sciences, where our main users are coming from our university's profile areas "Optoelectronics and photonics" and "Lightweight design with hybrid systems" (material sciences).



We leverage the synergies of these services and research to satisfy the needs of computational sciences while addressing the big challenges in computing systems research: energy efficiency, scalability and programmability.

Looking back at the development of HPC services during the reporting period, the path began with the successful procurement of the OCuLUS HPC system to establish ourselves as an HPC resource provider for Paderborn and local academic institutions, such as Bielefeld University and the Universities of Applied Science Bielefeld, Hamm-Lippstadt and Ostwestfalen-Lippe. About a third of the computing resources of our systems was allocated to users from other institutions in North Rhine-Westfalia.

Overall, the local demand for HPC resources continues to grow significantly. A key driver for this development is the increasing importance of computer simulation for researchers at Paderborn University. Within the reporting period several new projects (with an emphasis on highly parallel or distributed computing) have started. For example, DFG SFB/TRR 142, DFG SFB 901, ERC Starting Grant GreenOnWaterCat as well as additional DFG SPP, BMBF, BMWi and EU projects. The university has also hired new professors with working groups which make extensive use of computational methods.

Recently, two new research projects have been funded in which Professor Plessl's group collaborates with computational science groups in Paderborn. The goal of the DFG Project Perficien-CC is to analyze the most time-consuming codes running on the OCuLUS cluster and to accelerate the most suitable codes with FPGAs. The overarching objective of this effort is to

get empirical data about the suitability and potential of FPGAs for highly parallel, scientific applications. In the collaborative BMBF project HighPerMeshes, a domain-specific programming framework for specifying, compiling and executing unstructured mesh codes on heterogeneous cluster systems with CPUs, Manycores and FPGAs will be developed. Both projects comprise a close collaboration of Plessl's group with the groups of the PC² board members. Additionally, joint research proposals that strengthen the position of PC² as competence center that brings together expertise in computational science and innovative computer architectures are in preparation.

The availability of a powerful HPC infrastructure is crucial for the success of these researcher's projects. On the HPC operations side, the increased demand means that we will have to continue to scale up our HPC infrastructure in future, leading also to technical challenges for power supply and efficient cooling. From the research perspective, increased emphasis on computational methods offers interesting opportunities for joint research with computational scientists in collaborative research projects.

A continuing trend during the period was a growing demand for more diverse computing services beyond MPI-parallel jobs, such as high-throughput computing for serial jobs, big data jobs using Hadoop or Spark, or OpenStack cloud services. To support these needs we operate smaller HPC systems. For OpenStack applications we have procured a dedicated cloud computing cluster in 2016 jointly with IMT (the central IT services unit of Paderborn University). This well-established and successful cooperation with IMT also continued in other domains such as our campus-wide storage systems, identity management and vocational education.

During the reporting period, the management board has seen some turnover. Professor Franz Rammig and Professor Hans-Joachim Warnecke have retired. Professor Jens Förstner and Professor Thomas Kühne, whose research groups are very active users of our infrastructure, have been elected as new board members. Dr. Tobias Beisel has left after his graduation and Dr. Paul Kaufmann, Gavin Vaz and Harald Linden have been elected as the representatives of the scientific personnel and students, respectively replacing Maria Schütte, Dr. Jens Simon and Oliver Rabe. Professor Holger Karl has resigned as chairman of the board and is followed by Christian Plessl as chairman and Thomas Kühne as vice chairman.

Since the term of the advisory board ended in fall 2016, the advisory board also saw a significant change. The management board was fortunate to gain the following highly-qualified experts with diverse backgrounds to serve in the advisory board: Dr. Christoph Hagleitner, Volker Hamer, Professor Alexander Reinefeld, Dr. Marie-Christine Sawley and Dr. Felix Wolfheimer.

We would like to express our sincere thanks to all former management and advisory board members for their longstanding commitment and service to our institute. We hope to continue the friendly partnerships in the future.

Finally, several researchers working with PC² have successfully defended their dissertation. We congratulate Dr. Tobias Beisel, Dr. Tobias Kenter, Dr. Maria Schütte on this achievement.

HPC INFRASTRUCTURE PROVIDED BY PC²

The role of PC² as a center for high-performance computing is to coordinate the procurement and operation of central HPC systems and to make these systems available to scientists at Paderborn University and other research institutions in the state of North Rhine-Westfalia. The system administrators and technical advisers employed by PC² support researchers with using the HPC systems effectively and provide guidance with porting and optimizing their scientific codes.

The current main HPC system is the 10,000-core OCuLUS cluster which has been put in operation in 2013. In addition, PC² operates smaller, subsidiary HPC systems that are either dedicated for specific research projects or are customized to support workloads that do not fit the OCuLUS cluster, such as, big data, cloud or high-throughput computing applications.

An overview of our main computing systems that are currently in operation is shown in the tables on the right.

COMPUTING SYSTEM ACCESS

Academic users from North Rhine-Westfalia can apply for free of charge access to all publically available systems using the application form provided at the PC² website. The computing time allotment is assigned after a successful technical and scientific evaluation of a proposal for computing time. To support users that are new to HPC or that have low computing resource requirements, small allotments of computing time are assigned with an expedited technical review within a few days.

Access to dedicated purpose systems can be granted on a case by case basis. Users from commercial sites are also welcome but may have to pay a fee for using the systems.

FURTHER TECHNICAL INFORMATION AND APPLICATION FORMS

Additional technical information on the HPC infrastructure, installed software, access to the systems and computing time application forms can be found in the “HPC Services” section of the PC² website.

PRODUCTION SYSTEMS

NAME/ PURPOSE	SUPPLIER	YEAR OF INSTALL.	NUMBER OF NODES	NUMBER OF CORES	MEMORY PER NODE	PROCESSOR TYPES	INTER-CONNECT
OCuLUS Main HPC demand	Cluster-Vision	2013	616	9,920	64 GB, 256 GB, 1TB, 4 TB	Intel Xeon E5-2670, Intel Xeon E5-4670	InfiniBand QDR
Arminius+ Subsidiary HPC demand	Fujitsu	2010	60	720	36 GB	Intel X5650 2.67 GHz	InfiniBand QDR
High Throughput Cluster	Various	2009	–	650	up to 8 GB	Intel or AMD x86 64 bit	1G Ethernet
OpenStack Cloud	Teuto.net	2016	4	64	256 GB	Intel Xeon E5-2640v3	10 G Ethernet
Big Data	Cluster-Vision	–	80	320	32 GB	Intel Xeon E3-1240v3	10 G Ethernet

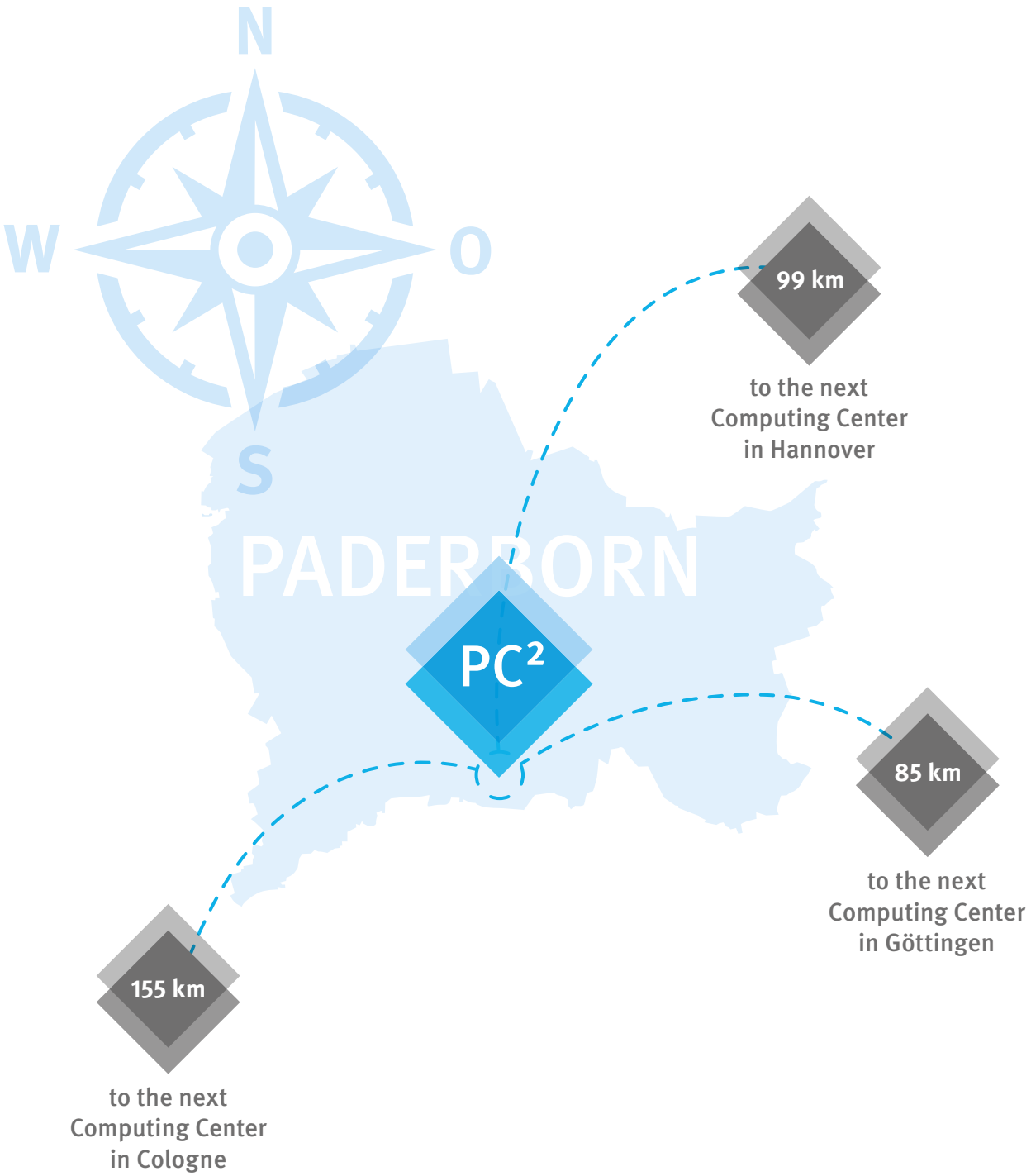
RESEARCH SYSTEMS (SELECTION)

NAME/ PURPOSE	YEAR OF INSTALL.	CPU	ACCELERATORS	SOFTWARE STACK	TECHNOLOGY
XCL Cluster	2016	Xeon E5-1630v4	Xilinx Virtex-7 VX690T + Xilinx Kintex UltraScale KU115 FPGAs	Xilinx OpenCL toolfow (SDAccel)	8-node cluster with 2 FPGA cards per node (AlphaData ADM-PCIE-7V3 and AlphaData ADM-PCIE-8K5)
Maxeler MPC-C	2012	Xeon X5660	Xilinx Virtex-6 SX475T	MaxCompiler (data flow language)	4 PCIe FPGA boards, MaxRing interconnect
Intel HARP2 Cluster	2017	Xeon Broadwell	Intel/Altera Arria 10	Altera OpenCL and HDL toolfow, Intel AAL	10-node cluster with hybrid Xeon/ FPGA multi-chip package processors with QPI interconnect

STORAGE SYSTEMS

TYPE	SUPPLIER	YEAR OF INSTALL.	CAPACITY	FILE SYSTEMS	AVAILABILITY
Network Attached Storage	Isilon	2009	54 TB	NFS, CIFS	all systems
Parallel File System	ClusterVision	2013	500 TB	BeeGFS	OCuLUS

FACTS AND FIGURES


N
W
O
S
PADERBORN
PC²
99 km
to the next
Computing Center
in Hannover
85 km
to the next
Computing Center
in Göttingen
155 km
to the next
Computing Center
in Cologne

BODIES

MANAGEMENT BOARD

The PC² is headed by an interdisciplinary board comprising professors from various working groups of Paderborn University. The following people were appointed as PC² management board members as of January 2017.

Prof. Dr. Michael Dellnitz
Department of Mathematics

Prof. Dr. Jens Förstner
Department of Electrical Engineering

Prof. Dr. Holger Karl
Department of Computer Science

Dr. Paul Kaufmann
Department of Computer Science
Representative of scientific personnel

Dipl.-Inf. Axel Keller
Paderborn Center for Parallel Computing
Representative of technical and administrative personnel

Prof. Dr. Thomas D. Kühne (Vice Chairman)
Department of Chemistry

Harald Linden
Student representative

Prof. Dr. Torsten Meier
Department of Physics

Prof. Dr. Burkhard Monien
Department of Computer Science (Emeritus)

Prof. Dr. Gudrun Oevel
Representative of the University's central IT services unit (IMT)

Prof. Dr. Marco Platzner
Department of Computer Science

Prof. Dr. Christian Plessl (Chairman)
Department of Computer Science

Prof. Dr. Wolf Gero Schmidt
Department of Physics

M.Sc. Gavin Vaz
Paderborn Center for Parallel Computing
Representative of scientific personnel

Prof. Dr. Jadran Vrabec
Department of Mechanical Engineering

Prof. Dr. Andrea Walther
Department of Mathematics

ADVISORY BOARD

To promote its trans-regional character, the PC² management board is supported by an advisory board. The advisory board is filled with representatives of science, industry and ministerial administration, providing professional insight for strategic decisions.

Dr. Christoph Hagleitner
Manager Accelerator Technologies
IBM Research Zurich, Switzerland

Volker Hamer
Head of Dept. Scientific Infrastructures and IT
NRW Ministry for Innovation, Science and Research, Düsseldorf, Germany

Prof. Dr. Dominik Marx
Institute for Technical Chemistry
Ruhr-University, Bochum, Germany

Prof. Dr. Alexander Reinefeld
Scientific Director
Zuse Institute, Berlin, Germany

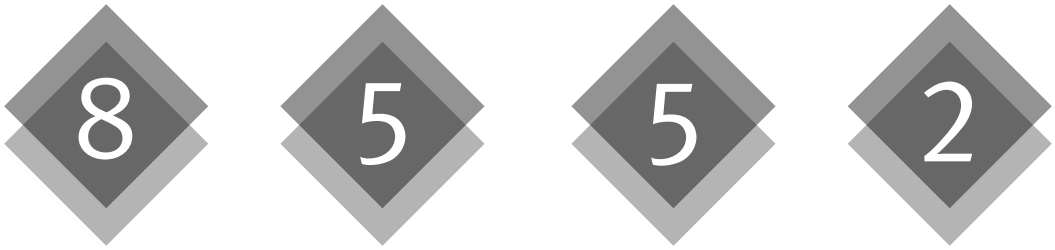
Marie-Christine Sawley, PhD
Director Exascale Computing Research Lab
Intel, Paris, France

Prof. Dr. Wilhelm Schäfer
President Paderborn University
Paderborn, Germany

Dr. Felix Wolfheimer
Manager High-Performance Computing
CST – Computer Simulation Technology AG
Darmstadt, Germany

PC² STAFF

In the years 2015 and 2016, the PC² employed



research associates

administrative and technical staff

trainees

students and graduate assistants

Justin Amedick

Dipl.-Inf. Bernard Bauer

Dr. Tobias Beisel

Fabian Berendes

Philipp Borkowski

Birgit Farr

Dr. Server Kasap

Dipl.-Inf. Axel Keller

Michaela Kemper

Dr. Tobias Kenter

Dipl.-Ing. Andreas Krawinkel

M.Sc. Michael Laß

Claudia Mergard

Holger Nitsche

Prof. Dr. Christian Plessl

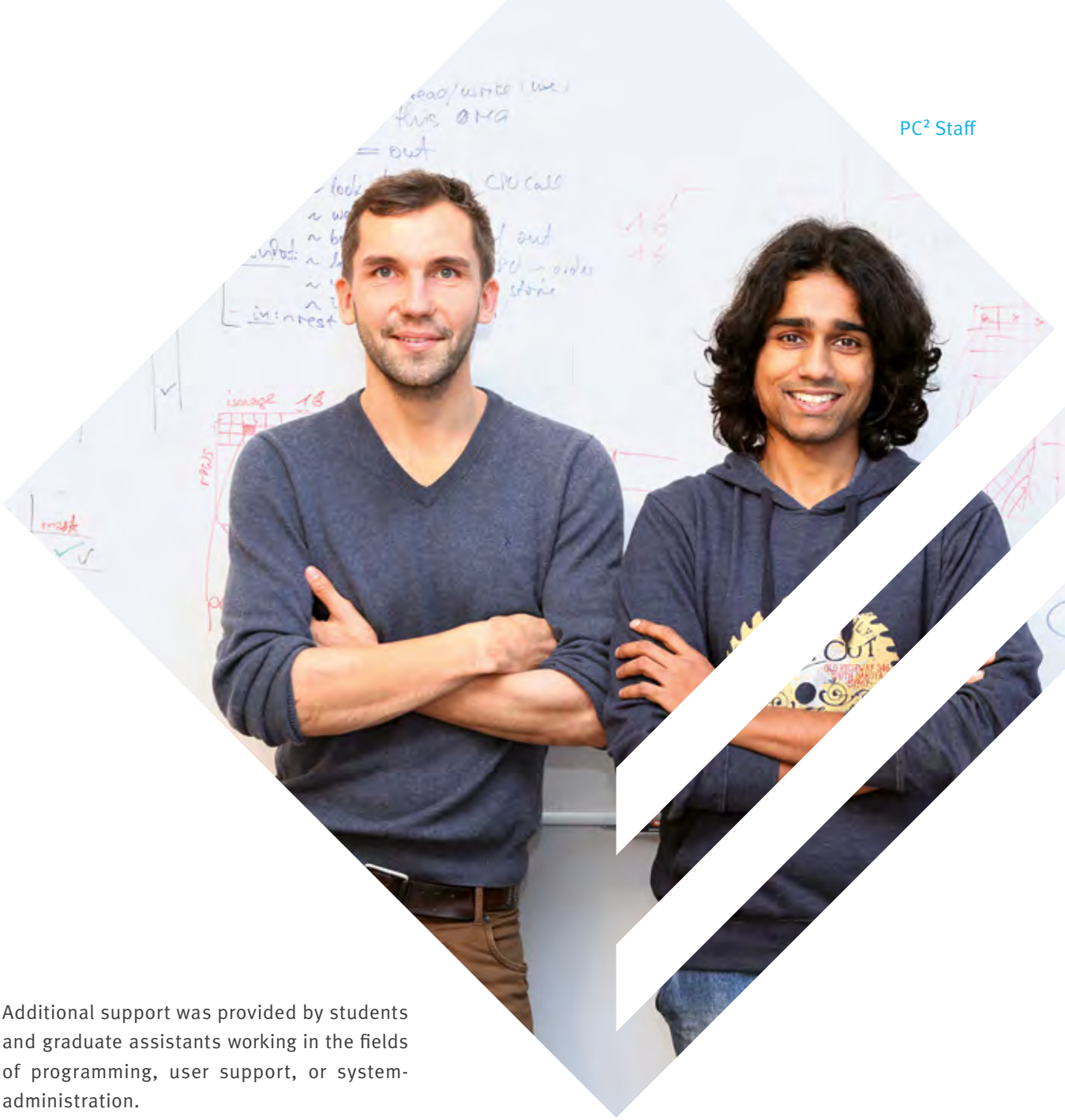
M.Sc. Heinrich Riebler

Dr. Maria Schütte

Dr. Jens Simon

M.Sc. Gavin Vaz

Nils Winnwa



Additional support was provided by students and graduate assistants working in the fields of programming, user support, or system-administration.

Johannes Schuster

Abdul Sami Nassery

Oliver Mangold

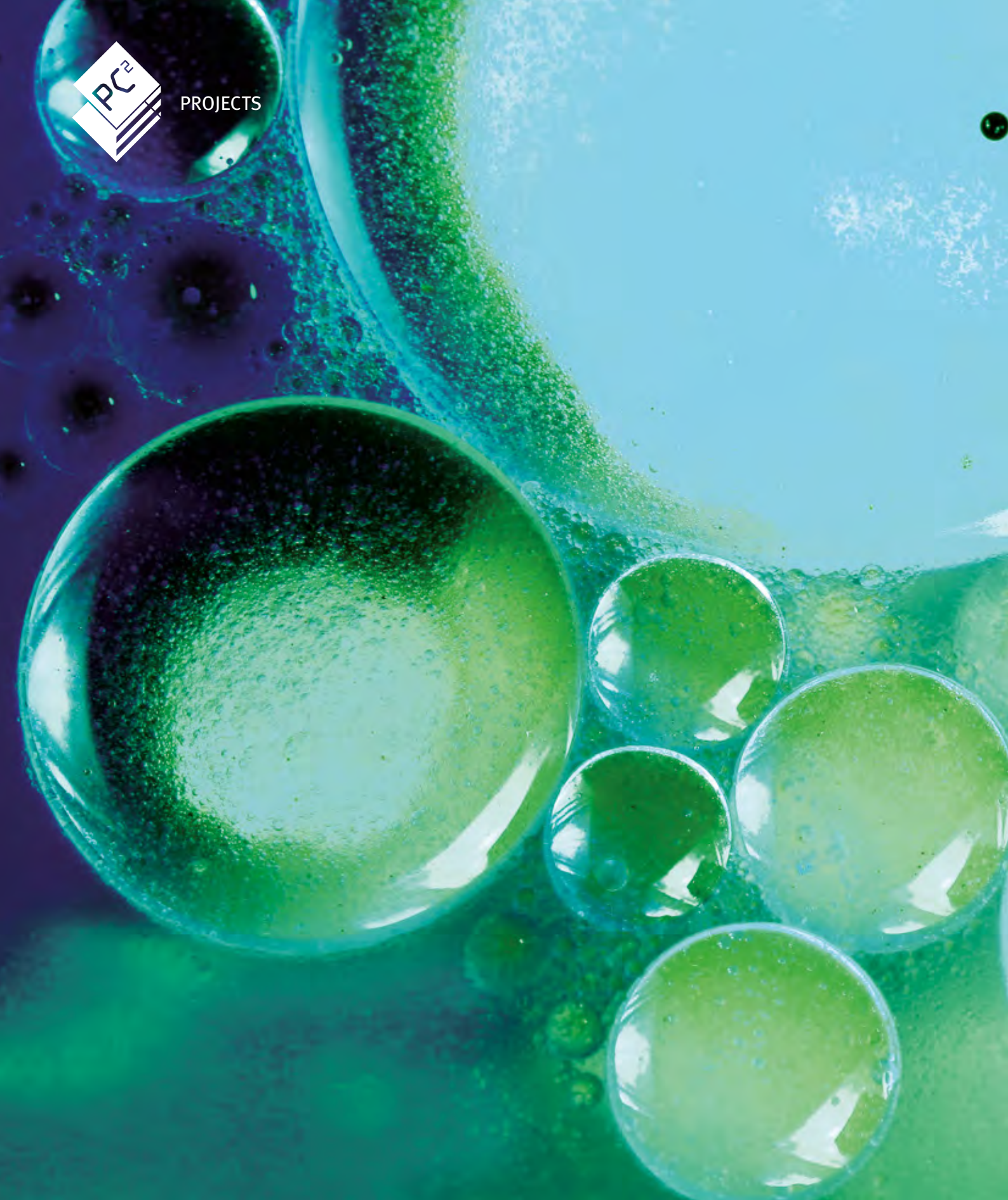
PROJECTS

RESEARCH PROJECTS

Our HPC systems and HPC user advisors provide computing resources and consulting for the projects of a large number of researchers from Paderborn University, local academic institutions and other universities in North Rhine-Westfalia. The main computing resource used by these projects is our HPC cluster OCuLUS. This system offers a maximum performance of more than 200 TFlop/s, that is, 200 trillion floating-point computations per second. During the reporting period, the use of OCuLUS was instrumental for the research in more than 50 third-party-funded projects, for example, the DFG-funded projects SFB/TRR 142, SFB 901, GRK 1464, FOR 1405, DFG FOR 1700, or the BMBF-funded projects SkaSim and HPC-FLiS. OCuLUS has also been used for more than 20 projects by external users.

Overall, the results achieved in these projects have been received very positively by the scientific community. Just for the top 20 of our users alone, the research enabled by our infrastructure has led to the publication of more than 260 peer-reviewed articles in leading journals and conference proceedings, for example, Nature Communications, Physical Review B, or Journal of Physical and Chemical Reference Data. Also, this research contributed to the qualification of young scientists and led to the completion of 27 PhD dissertations, 42 Master's and 38 Bachelor's theses.

To provide some insight into the variety of this research, we present a cross-section of projects that have been enabled by our HPC systems and consulting by our HPC experts in the following.


PROJECTS


5X/0.15
10X/0.30
THERMO-
DYNAMICS

The Chair of Thermodynamics and Energy Technology of the Paderborn University (ThEt) has a longstanding experience in the field of molecular modeling and simulation. Work has been funded primarily by Deutsche Forschungsgemeinschaft (DFG) in different Collaborative Research Centers (SFB 412, SFB 716), a Priority Program (SPP 1155) and a Transfer Unit (TFB 66). ThEt has developed molecular force field models for numerous compounds that are in the focus of the chemical industry. These models were applied for the prediction of thermophysical properties, with an emphasis on vapor-liquid equilibria, considering very large sets of systems.

INTERVIEW

Patrizia Höfer met with Professor Jadran Vrabec, Andreas Köster and Dr. Gábor Rutkai to discuss their research approach and objectives.

PH: WHAT IMPORTANT ASPECTS OF THERMODYNAMICS RELATE TO YOUR RESEARCH PROJECT?

First, we must bear in mind that thermodynamics is an old branch of physics. It was developed while seeking to understand the steam engine, so it is around 200 years old. By the end of the 19th century, it was generally believed that the formalisms, such as conservation of energy and the definition of entropy, had all been worked out.

M.Sc. Andreas Köster

Andreas Köster has been working as a research assistant and PhD student since 2013 in the Thermodynamics and Energy Technology group chaired by Prof. Dr. Vrabec. In addition to determining material properties using force-field-based multibody simulations, he is involved in method development and programming. He has already written 17 papers on molecular simulation.

But what still remained, and in fact will remain for the foreseeable future, is that we also have to understand the properties of materials. We have to quantify the properties of the materials involved in processes. If you look at what has been quantified by experiments over the past 200 years, you will notice that data availability is very spotty. Given so many different substances and their potential to form mixtures, as we know so well from the chemical industry for example, we need new methods that will characterize these materials more efficiently than before. So, we are trying to take a non-experimental approach and to obtain these results theoretically via simulation.

PH: WHY DO YOU CHOOSE MOLECULAR MODELING FOR YOUR INVESTIGATIONS?

Conventional experimental methods are laborious, expensive and time-consuming. Our method is also not brand new, but it follows a different approach. We know from physics that materials behave in specific ways because of the molecular interactions. Rather than describing the behavior of the material, we describe the molecules' interactions, in particular among themselves, using physically based potential functions. We obtain the parameters for those functions from quantum mechanical calculations, in part. Working from the existing data on a molecule, such as its polarity or a geometry, we create a so-called force field model. Once everything has been written out and parameterized, we can use this model to calculate all thermodynamic properties.

This method originated in the 1950s when the first computers became available. The first molecular simulations were run in 1953. Before then, physicists were able to develop the underlying methods but could only solve them for very simple models. With the power of computers growing exponentially, molecular modeling went from being a niche field to a truly exciting, major field of research.

Prof. Dr.-Ing. habil. Jadran Vrabec

Jadran Varbec is the Chair in Thermodynamics and Energy Technology at the Faculty of Mechanical Engineering (since 2009). His research focuses are molecular modeling and simulation, applied experimental thermodynamics and energy technology.

PH: WHAT DO YOU NEED TO RUN SIMULATIONS WITH THIS KIND OF MODELING?

There are various prerequisites for this kind of simulation. First, we need a very powerful computer because the equations, which stem from Boltzmann's definition of entropy, are not analytically solvable. We have even formed a society – the "Boltzmann-Zuse Society for Computational Molecular Engineering" – in honor of Boltzmann as the man of molecules and Zuse as the pioneer of programmable computers. These two never met in person, but it was only through the efforts of both that Boltzmann's equations ever became solvable.

Another prerequisite are the simulation programs. We are working in this field here in Paderborn. There are commercially available programs, but we prefer not to use them because it is like working with a black box. Instead, we develop our own programs. We gain many more exciting insights working on our own tools. Of course, a challenge in all this is ensuring that our own tool does its job properly. There are currently two major programming projects running in cooperation with other universities, i.e. TU Kaiserlautern, TU München and the University of Stuttgart, the results of which have already been published and are available as open source. My aim and ambition is to enable doctoral students to do their own significant research, so that they can be much deeper involved than just users.

In short: we need theory, computers, simulation programs and interesting questions.

PH: WHERE DO THESE MODELS AND THE RESEARCH PROJECT AS A WHOLE STAND WITH RESPECT TO MODERN INDUSTRY?

The chemical process industry uses many different material combinations in production. Working with these various mixtures requires thermophysical property data. Companies like BASF or Bayer are particularly interested in ex-

Dr. Gábor Rutkai

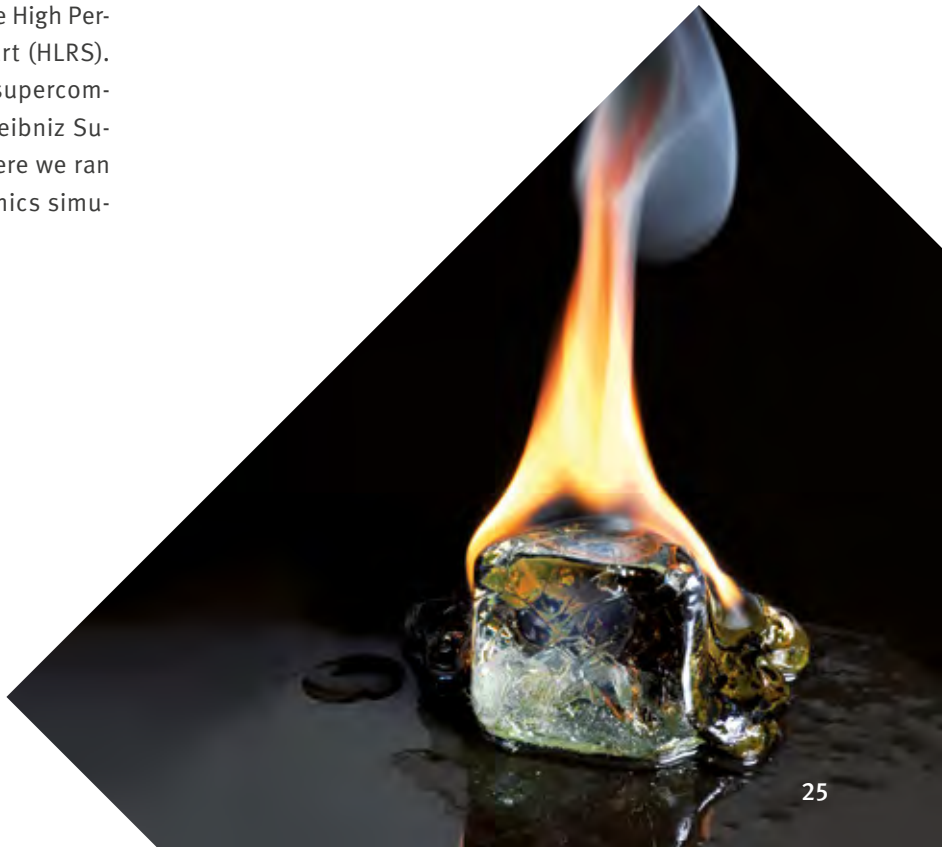
Gábor Rutkai has been working as a research assistant in the Department of Thermodynamics and Energy Technology at the Faculty of Mechanical Engineering since 2010. Among other things, his tasks include adapting equations of state using experimental and simulation data and analyzing thermodynamic processes.

perimentally obtained data that can be guaranteed as reliable results. But other classical predictive methods are also used to obtain such data. Molecular modeling and simulation is one component in this field. Unfortunately, the prevailing attitude towards this method is still relatively conservative, especially in Germany.

Molecular modeling and simulation is used much more heavily in biotechnology. There has been a series of industrial projects in my field of research, which speaks for a fundamental interest in the method.

PH: HOW DO YOU MAINTAIN HIGH COMPUTING POWER?

At most times, we have several strings to our bow. One is our collaboration with the High Performance Computing Center Stuttgart (HLRS). However, we have access to other supercomputers as well, for example at the Leibniz Supercomputing Centre in Munich, where we ran the world's largest molecular dynamics simulation in 2013. PC² in Paderborn is especially important to us for a number of reasons. The computer is extremely comfortable compared to other computers in the country. By this, I mean PC² affords a great deal of flexibility when it comes to the length of our simulation jobs, for example. In the researcher's daily routine, the local machine is the most comfortable one because its operation has been optimized to serve the users. As a member of the board, I am very happy with our computing center in Paderborn. Working with such a computing center is efficient because around 90% of the scientific simulations are practically made to run on the PC², with its OCuLUS cluster and workload manager.




ALCHEMICAL
MOLECULAR
SIMULATIONS

Molecular simulations serve to provide unique insights at the atomic scale. A typical application is simulating the process of a drug binding to the active site of a medically relevant enzyme. In developing new, more potent active compounds, the type and strength of atomic interactions are the central basis from which to make further optimizations. Even nowadays, it is still a major challenge, scientifically and technologically, to predict and accurately quantify these interactions.

We use molecular dynamics simulations to determine these binding energies (see Figure 1). While simulations like these typically scale on supercomputers such as OCuLUS at PC² with O(n log(n)), the umbrella sampling and free energy perturbation methods we employ allow one to divide a simulation of the change between 'bound' and 'unbound' state into separate, independent simulations. This 'alchemical' approach allows far higher parallelization and thus more efficient use of computing resources, thus making processes quantifiable that would otherwise be poorly accessible in experiments.

Our current research relates to ion channels and other membrane proteins, and the stability of protein–protein complexes. Focus is specifically on modulation, or in other words targeted stabilization or destabilization.

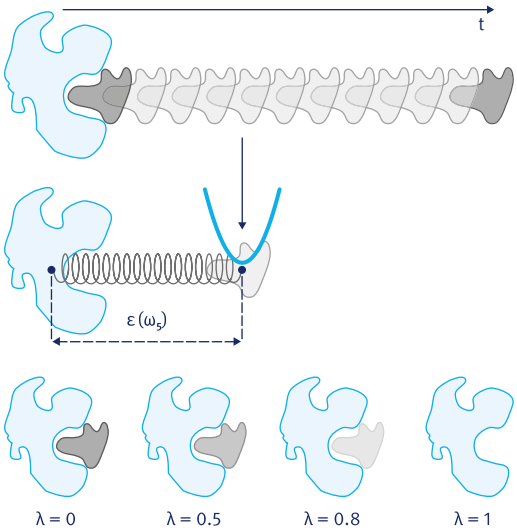


Fig. 1: Various methods are used to simulate molecular interactions. Illustrated on the top is the principle of umbrella sampling, where individual simulations are run along a given reaction coordinate. Shown below is the concept of free energy perturbation, where a system is 'alchemically' transformed from one state (bound) to another (unbound).

Dr. Jens Krüger

Jens Krüger has been working as a researcher and habilitand in the Applied Bioinformatics Group of Oliver Kohlbacher at Eberhard Karls Universität Tübingen from 2011 to 2016. Since 2017 he has been leading the High Performance and Cloud Computing Group at the IT Center of the University of Tübingen. Besides improving accessibility of simulation methods and computing resources via science gateways, he works mainly on modeling and simulating biological membranes, proteins and ion channels. For this, he uses supercomputers such as OCuLUS at PC².


SIMULATIONS
OF STRUCTURED
PACKINGS WITH
COMPUTATIONAL
FLUID DYNAMICS

The general goal of chemical engineering is to achieve increased efficiency and capacity of separation units at the lowest possible costs. This has brought about a novel generation of column internals which provide enhanced mass transfer performance and relatively low pressure drops. Among these internals, regular corrugated packings, also referred as structured packings, have gained wide acceptance. Over the years, efforts have been made toward the choice of an appropriate packing material and optimization of the corrugated sheet geometry – achieved only if flow structures and transport phenomena in packings are properly captured.

In the last few decades, Computational Fluid Dynamics (CFD) methods have become an efficient tool, augmenting the greater knowledge of the fluid dynamics in structured packings, substantially reducing the need of experimental efforts. The simulation of an entire column requires an intense computational effort, meaning CFD simulations being applied to only relatively small representative elements of structured packings. But even small elements, with dimensions of about 3x3x3 cm, must be subdivided into approximately 20 million cells. This requires significant computational power, and simulations must be carried out in parallel on multiple cores ranging from 128 to 512, and taking several weeks to complete. Consequently, we exploit the OCuLUS cluster every day, which is essential for the success of our projects. As simulation tools, we use the commercial CFD software Star-CCM+ and the open source CFD-code OpenFOAM.

Prof. Dr.-Ing. habil. Eugeny Kenig

Eugeny Kenig is head of the Fluid Process Engineering and the Chairman of the Management Board for the Competence Center for Sustainable Energy Technology at Paderborn University. He put forward the concept of complementary modeling based on a combination of approaches with different detailization degrees. He is active in the optimization of column internals applied in industry, where the advantages of Computational Fluid Dynamics are widely used.

PROJECTS


MAGNETIC FINGERPRINTS OF INTERFACE DEFECTS IN SILICON SOLAR CELLS

In principle, silicon-based solar cells are capable of converting up to 30 percent of sunlight to electricity. Even under ideal lab conditions, however, different kinds of loss mechanisms limit the conversion. In particular, defects and grain boundaries – where electrons and holes meet – are one source of energy loss. This issue is addressed in so-called heterojunction cells by an ultrathin layer of disordered amorphous silicon that is deposited on top of crystalline silicon. This thin film saturates many interface defects and conducts charge carriers out of the cell.

Heterojunction solar cells have shown high efficiency factors of more than 25 percent [1]. To increase their efficiency further, the challenge lies in better understanding the processes at the remaining interface defects.

Experimental and theoretical physicists from the Helmholtz Zentrum Berlin and Paderborn University have managed to use the electron spin, i.e., the inherent magnetic moment of the electrons, as probe for the local atomic structure of interface defects. By using electrically detected magnetic resonance (EDMR), they were able to detect specific signatures related to local defects' structure by measuring the magnetic fingerprint in the photo current of the solar cell under a magnetic field and microwave radiation [2]. But how can these signatures in the photo current be used to better understand the loss mechanisms in the solar cells?

Large-scale computer simulations of the structure, electronic properties and magnetic response of the c-Si/a-Si:H interface performed at the Paderborn PC² come into play. Density-functional theory (DFT) was used to develop microscopic models for the a-Si:H/c-Si interface between the hydrogenated amorphous and crystalline silicon material in the solar cell. Examples for interface models derived from the DFT calculations are shown in Fig. 2. The realistic modeling of the amorphous material –

Prof. Dr. Wolf Gero Schmidt

Wolf Gero Schmidt has been heading the Theoretical Material Physics Group at Paderborn University since 2006. Previously, Schmidt worked, inter alia, at the Massey University in Auckland, New Zealand. Current research areas include theoretical description and numerical modeling of optical and electronic excitations in semiconductors and ferroelectrics, mesoscopic electron transport and phase transitions in low-dimensional systems.

which lacks long-range order and needs to be modeled with very large supercells – was one of the technical challenges, and could only be met by using massively parallel high-performance computing resources.

Electrons occupying interface defect states interact via their spins, i.e., their small magnetic moments, with the electrons that occupy the chemical bonds in the environment of these defects. Highly specific coupling scenarios occur due to specific strengths and orientations of the electron orbital angular momentums and spin angular momentums, characterizing the various defect structures.

This effect can be mathematically described by a so-called g-tensor, a quantity which is:

I. highly defect-specific in that it has fingerprint character,
II. can be measured by EDMR, and
III. is determined by the local atomic and electronic structure.

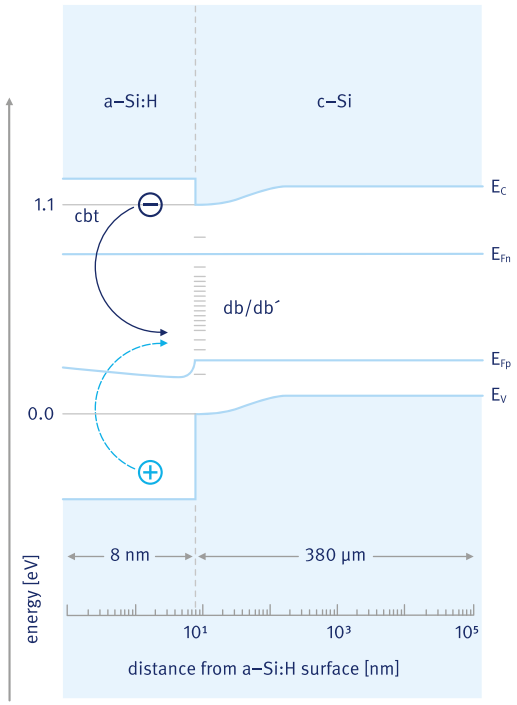


Fig. 1: Qualitative energy band diagram of the a-Si:H/c-Si heterointerface with applied forward bias. EC (EV), EFn (EFp) mark conduction (valence) band edges and electron (hole) quasi-Fermi levels, respectively.

Dr. Uwe Gerstmann

Uwe Gerstmann joined the Material Physics Group at Paderborn University in 2010. Previously, he worked at the Université Pierre et Marie Curie in Paris. Gerstmann's primary research interest is with the influence of point defects and relativistic effects on the electron structure of semiconductors and metals.

The latter point was exploited to determine the g-tensor starting from the output of the DFT calculations: The Paderborn theory group has developed and implemented efficient schemes to numerically calculate the g-tensor [3,4]. Based on these schemes, g-tensor calculations were performed for a-Si:H/c-Si interface defects, and compared with the magnetic signatures detected in the solar cell photo current.

Based on the comparison between experiment and theory, the most relevant defects at the a-Si:H/c-Si interface could be identified and the performance-limiting charge recombination processes were revealed in microscopic detail. After tunneling into the a-Si:H layer, excess electrons from the c-Si wafer will be captured in conduction band tail states (cbt in Figs. 1 and 2). Subsequently, the electrons tunnel into energetically lower lying dangling bond states (db and db' in Figs. 1 and 2). Once a dangling bond state is doubly occupied, spin-independent capture of a hole below the quasi-Fermi level EFp completes the recombination step. For the first time ever it has become possible to directly detect and characterize the processes, with atomic resolution, that compromise the solar cells' high efficiency. These findings will help to further optimize solar cells and decrease production costs. The methodology and numerical tools developed here are not limited to a-Si:H/c-Si interfaces. They may also be used to map paramagnetic states involved in spin-dependent transport in organic or other inorganic materials, thereby providing general insight into device limiting states and processes.

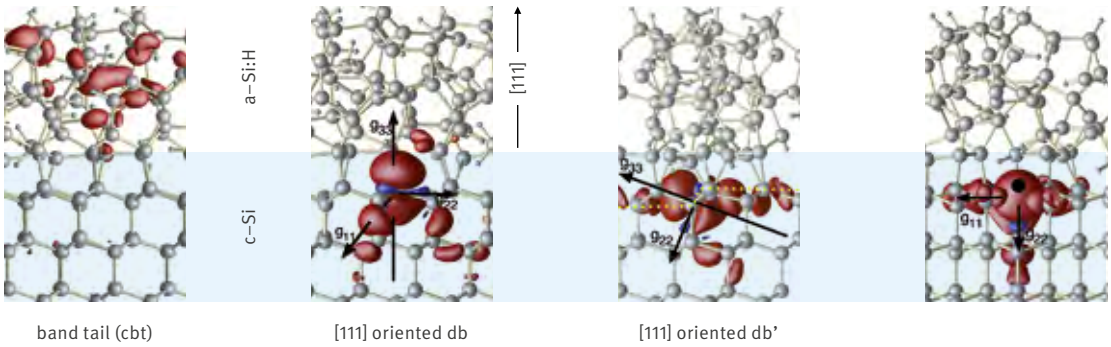
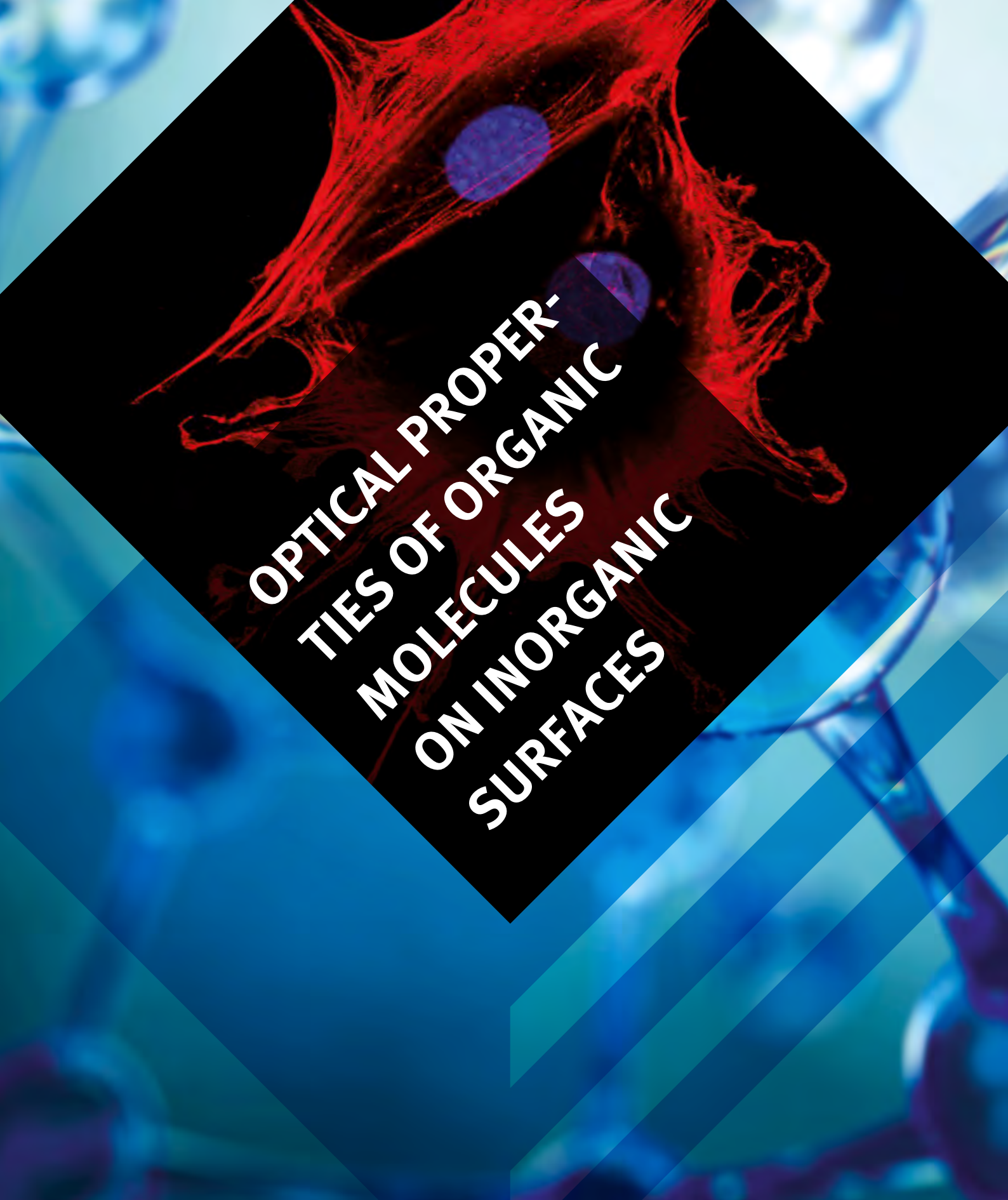


Fig. 2: Calculated microscopic atomic structure and magnetization density (red: positive, blue: negative) for recombination-active structures: (a) prototype conduction band tail, (b) Pb-like [111]-oriented dangling bond (db) at the heterojunction, and (c) a tilted, 110 degree off-axis oriented dangling bond (db') at a microstep of monatomic height (dotted line). Large spheres: Si, Small spheres: H.

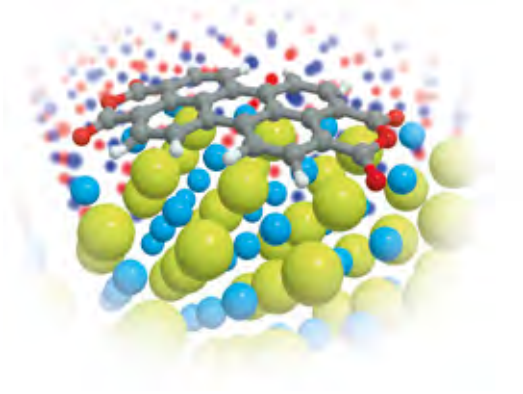
Photovoltaic system of 4,570 square meters on the roof of the Benteler Arena in Paderborn can provide 600 MWh, i.e. the annual demand of nearly 200 households. Many of these systems could be replaced by more efficient ones.

Photo: Jörn Hannemann/WESTFALEN-BLATT


OPTICAL PROPERTIES OF ORGANIC MOLECULES ON INORGANIC SURFACES

In modern electronic devices, organic molecules are deposited on inorganic surfaces. Tailoring their optical properties through lateral and adsorbate-substrate interaction is a prerequisite for obtaining more efficient organic light emitting diodes and organic photovoltaic cells. Computer simulations have become an indispensable tool for predicting absorption and fluorescence spectra of dye molecules. A particular challenge is the quantum-chemical treatment of quasi-periodic systems such as adsorbate-surface systems. As a reference system, which is also studied experimentally by the Sokolowski group in Bonn, we investigated the PTCDA molecule adsorbed on surfaces of sodium chloride. Calculations of large systems in a reasonable timescale, (i.e., applying first-principles methods based on density functional theory) are only possible on large-scale computer clusters.

In this research project, we study the optical properties of the PTCDA molecule adsorbed on surfaces of sodium chloride crystals with quantum-chemical methods. We focused on a theoretical analysis of the influence of the PTCDA-surface interaction on optical properties by applying time-dependent density functional theory.



Two main effects are responsible for the observed red shift of the excitation energy [1].

First, molecular orbital energies are shifted by the electrostatic potential of the surface. Second, the molecular geometry is distorted by an interplay of attractive and repulsive forces between the surface and the molecule (see illustration).

For the PTCDA-NaCl system the effects are relatively small. In order to identify possible photoswitchable systems we are exploring in silico chemical modifications of the PTCDA molecule that increase the sensitivity of the molecule's optical properties to the underlying surface.

Prof. Dr. Thomas Bredow

Thomas Bredow is member of the Mulliken Center for Theoretical Chemistry within the Institute of Physical and Theoretical Chemistry at the University of Bonn. His main field is solid-state quantum chemistry. He focuses on developing of theoretical models for heterogeneous catalysis, photocatalytic water splitting, and ion batteries, in close cooperation with experimentalists. He applies quantum-chemical methods ranging from semiempirical and density-functional theory to linear-response perturbation theory.

PROJECTS


MOLECULAR
DYNAMIC
STUDIES

The geometric increase in computer performance over the past few decades, along with advances in applied physics and mathematics, has led to the birth of a new way of doing science. Right at the intersection of theory and experiment, computational science allows for computer experiments under controllable and reproducible conditions. In this way, computer simulations have been successful in explaining a large variety of physical phenomena and have guided experimental work.

In addition, it is even possible to predict new phenomena by conducting experiments in silico that would otherwise be too expensive, difficult or simply impossible to perform. But the most invaluable outcome of computer simulations is by far the insight they provide into system behavior and dynamics.

The two most common computational techniques for this area of study are the Monte Carlo and the molecular dynamics (MD) algorithm [1]. The latter is simply the numerical solution of Hamilton's equation of motion, which allows both equilibrium thermodynamic and dynamic properties of a system to be computed (at finite temperatures). It additionally provides a window into real-time evolution of atoms and serves as a computational microscope.

AB-INITIO MOLECULAR DYNAMICS

One of the most challenging but essential aspects of MD simulations is the calculation of interatomic forces. In classical simulations they are computed from empirical potential functions, which have been parameterized to reproduce experimental or accurate ab initio data of small model systems.

Although great strides in elaborating these empirical potentials have been made [2], the transferability to systems or regions of the phase diagram, different from the ones to which they have been fitted, may be restricted. Furthermore, they are unable to simulate chemical bonding processes (taking place in many relevant systems) with sufficient predictive power.

Prof. Dr. Thomas D. Kühne

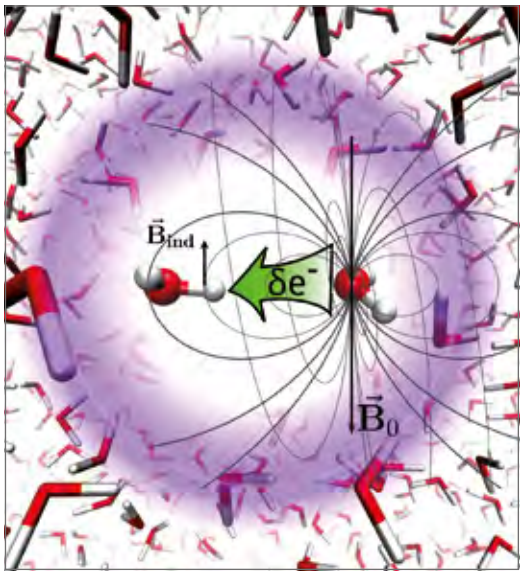
Thomas D. Kühne is currently a professor for "Theoretical Interface Chemistry" at the University of Paderborn. His research interests are the development of computational methods for ab-initio molecular dynamics and electronic structure theory, as well as the application of such techniques to investigate relevant questions of chemistry, condensed matter physics and material sciences.

Ultimately though, some of the most important and interesting phenomena of modern physics and chemistry are intrinsically non-classical.

A first principles-based approach, such as ab-initio MD (AIMD), where the forces are calculated on-the-fly from accurate electronic structure calculations, is quite attractive, since many of these limitations can be removed [3]. However, the increased predictive power and accuracy of AIMD simulations comes at a significant computational cost, necessitating the availability of massively high-performance parallel computing resources.

For this reason, density functional theory (DFT), to date is the most commonly employed electronic structure theory, but it is not without its faults. Nevertheless, the ab-initio approach is also not without problems – the relevant energy scale is tiny, well below k_BT, and in particular the attainable length and timescales are still one of its major limitations.

Therefore, the main focus of our research group is the development and application of novel AIMD methods of unprecedented efficiency and accuracy. In particular, the second generation Car-Parrinello AIMD method, which we developed, allows us to study phenomena that were previously thought unfeasible [4]. In spite of that, for large systems, the calculation of the total energy and the corresponding nuclear forces is still computationally expensive. This is due to the fact that solving the Schrödinger equation is a high-dimensional eigenvalue problem, whose solution requires diagonalization of the system's Hamiltonian, which typically scales cubically with its size. Thus, in order to circumvent this bottleneck, we recently proposed a new field-theoretic approach based on the grand-canonical potential for independent fermions, which scales only linearly with the size of the system [5]. In contrast to conventional DFT calculations, this development permits the study of very complex systems with up to a million atoms from first-principles. Moreover, for purposes of facilitating genuine quantum MD simulations, wherein the quantum-mechanical nature of the nuclei is explicitly taken into account, we also developed an efficient path-integral AIMD approach at essentially no additional computational cost, in comparison to the corresponding calculation using classical nuclei [6].

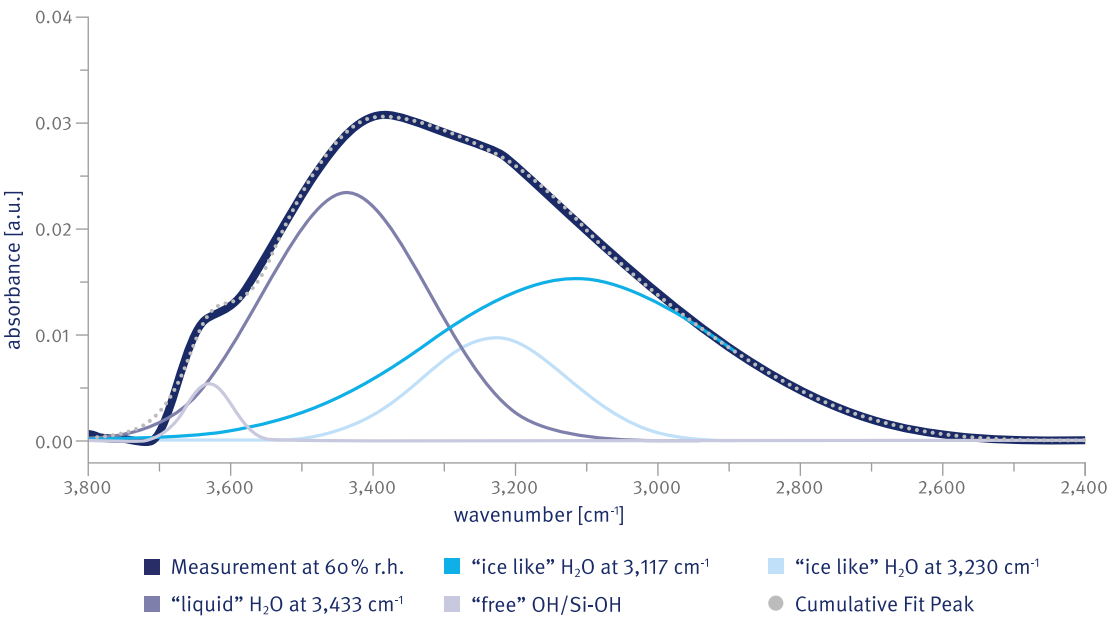


LARGE-SCALE APPLICATIONS

However, our emphasis is not solely on the development of new algorithms, but also on solving scientifically relevant questions of chemistry, physics, material sciences and biophysics. With regard of the latter, our current focus is on the structure and dynamics of complex systems in condensed phases. Specific examples are hydrogen bond networks in aqueous solution, biophysical reactions on water surfaces, and in confined geometries, but also solid/liquid interfaces, amorphous glasses and hydrogen-rich solids at high pressure. Moreover, we investigate the atomistic mechanism of non-volatile memory-devises, CIGS-based thin-film solar cells and proton exchange fuel cell membranes.

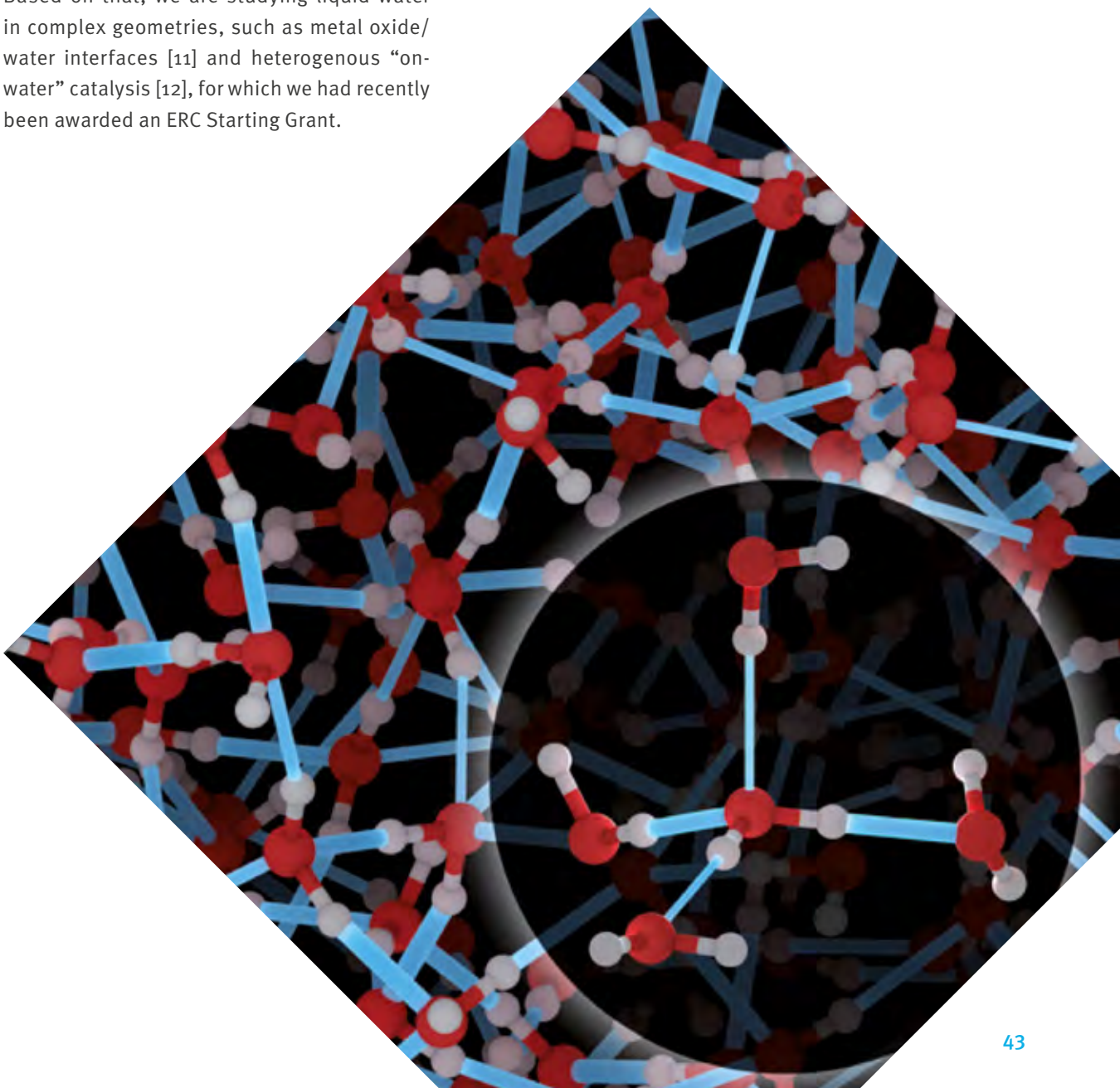
In the case of aqueous systems, we aim to understand the relationships between the structure and dynamics of the hydrogen bond network and spectroscopy. For instance, combining our recently developed energy decomposition analysis method [7] with second generation Car-Parrinello AIMD and XAS calculations, we have recently settled the longstanding controversy whether liquid water is coordinated in a four- or simply two-fold manner [8, 9].

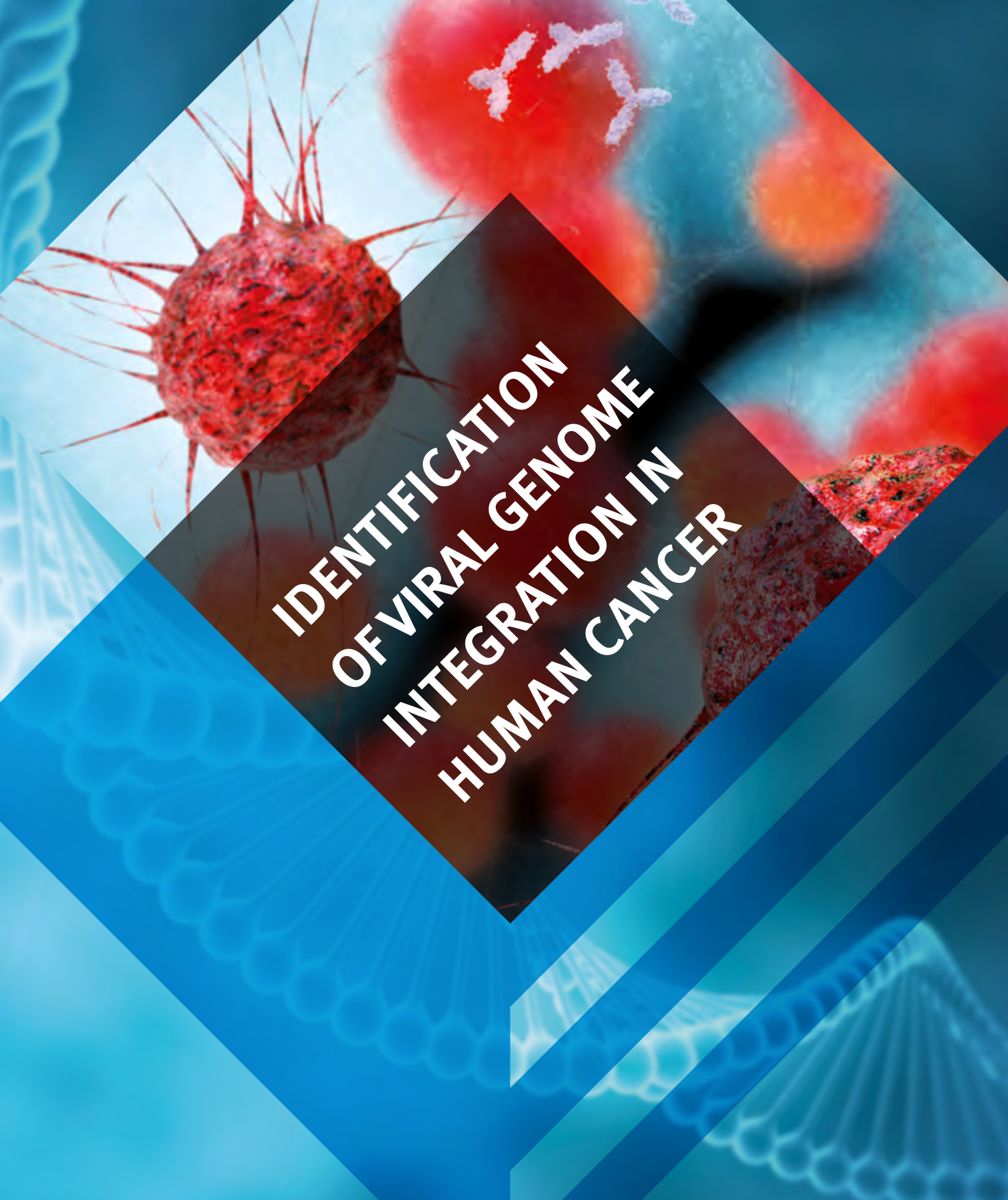
Furthermore, we have recently established a quantitative relationship between the anisotropy of the proton magnetic shielding tensor and the covalency of hydrogen bonding,



which leads to experimentally determine the strength of hydrogen bonding by means of NMR measurements [10].

Based on that, we are studying liquid water in complex geometries, such as metal oxide/water interfaces [11] and heterogenous "on-water" catalysis [12], for which we had recently been awarded an ERC Starting Grant.




IDENTIFICATION
OF VIRAL GENOME
INTEGRATION IN
HUMAN CANCER

Virus infections are estimated to account for up to 30 percent of all human cancers. Perhaps the best example in this context are infections with human papillomavirus, which causes uterine cervix cancer. Since 2006, a vaccine against HPV has been made available and for the discovery of this link, German researcher Professor Harald zur Hausen received the nobel prize in 2008.

Over the last decade, DNA from many tumors have been sequenced, but the role of virus infections remains largely elusive. Upon entry in human host cells, some viruses are able to integrate parts of their genome into the genome of the host cell, thereby changing the cellular programing and possibly turn the healthy cell into a tumor cell.

The research group is currently investigating into which regions of the human genome certain viruses are able to integrate their DNA and to understand what effects this has on the cellular program.

Sequencing data from tumors and normal tissue of the same patient, obtained from the American consortium “The Cancer Genome Atlas”, they are systematically screened for known pieces of around 5,000 viral strains and DNA insertions into localized host cells.

The systematic screening and analysis of these data requires significant computational power and storage, which is provided by the Paderborn Center for Parallel Computing.

PD Dr. Michael Nowak

Michael Nowak is group leader in the Institute of Pathology at the University of Bonn. His main research topics are the mechanisms of how tumors spread in prostate cancer and how these tumors inhibit the immune system.

INSIGHTS INTO THE ELECTRONIC STRUCTURE OF TYROSINASE

Hemocyanin transports dioxygen in arthropods and molluscs whereas tyrosinase furthermore transfers one oxygen atom subsequently to phenolic substrates, then oxidizes the catechols to quinones.[1] Tyrosinase is also involved in melanin production for skin, hair and feathers and in browning processes of fruits. Studying these metalloproteins allows us to harness their activation principles for future biomimetic catalysts.

The Herres-Pawlis group explores biomimetic catalytically active model complexes [2, 3]. Through a multi-method approach, the group applies techniques such as low-temperature stopped-flow, resonance-Raman, XAS and EPR spectroscopy, voltammetric methods and spectroelectrochemistry. Importantly, full-simulation of all reaction steps by density functional theory (DFT) calculations are performed to support the results of the utilized spectroscopic techniques and to understand the mechanisms behind them.

A comprehensive theoretical analysis of the conformers of a real-life peroxo-dicopper(II) species (see figure) displays catalytic reactivity [4]. Geometry optimizations and TD-DFT calculations proved to be robust in the prediction of the experimental data. For a correct description of the energetics, empirical dispersion with Becke-Johnson damping, a PCM solvent model and a 3ζ basis set are required. Through NBO analysis, they elucidated the donor competition between pyrazolyl and pyridinyl moieties and the CDA analyses gave insights into the electronic structure of the real-life peroxo species.

These insights into the model complexes and their reactivity require a fundamental and tedious DFT study. Furthermore, the quantum chemical code requires significant long-running calculations (7–21 days).

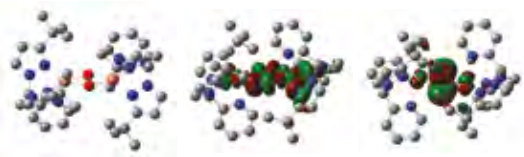


Fig.: left: Bis(pyrazolyl)methane stabilized peroxo-dicopper complex; right: lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO)

Prof. Dr. Sonja Herres-Pawlis

Sonja Herres-Pawlis holds the chair for Bioinorganic Chemistry at RWTH Aachen University. She is currently speaker of the interdisciplinary DFG-research unit FOR 1405 and has published more than 120 original papers and four patents.

Dr. Alexander Hoffmann

Alexander Hoffmann holds a permanent position the Herres-Pawlis group for DFT, X-ray crystallography and special spectroscopic methods. He is coordinator of the DFG-research unit FOR 1405 “Charge transfer dynamics in bioinorganic copper complexes.”


INVESTIGATION
OF PHOTONIC
STRUCTURES

Within the last decade the research field of Optoelectronics and Photonics has emerged as an active and successful focal area at the Paderborn University. Some highlights investigated are novel light diodes & lasers, ultrafast digital communication via fibers, integrated optical circuits, biological photonic structures, concepts for optical quantum computers, optical sensors, antennae for light, metamaterials, and holograms from ultrathin layers.

The fundamental interplay of light and matter in nanostructures has been investigated at the Paderborn University for a long time. In addition to the many individual projects and bilateral cooperations, several large-scale joint projects have resulted since the "Center for Optoelectronics and Photonics Paderborn (CeOPP)" was established in 2006. In 2008, a DFG graduate school involving 15 research groups and 26 PhD students working on the topic of "Micro- and Nanostructures in Optoelectronics and Photonics" began, and established in 2013 a DFG SFB/Transregio on "Tailored nonlinear photonics: From fundamental concepts to functional structures" together with TU Dortmund.

Embedded into this fruitful research environment, Professor Jens Förstner's group, uses theoretical models and numerical simulations to investigate photonic structures, often in close collaboration with the many world-class experimental groups at Paderborn University and external partners.

Prof. Dr. Jens Förstner

Jens Förstner, head of the Theoretical Electrical Engineering (TET) group at Paderborn University, studied Physics and Computer Science at Philipps Universität Marburg and University of Kent at Canterbury/UK. During his PhD at Technical University Berlin and later for postdoctoral studies at University of Arizona, where he focused on simulating nanophotonic structures, Förstner led an Emmy Noether research group on "Computational Nanophotonics" in Germany and was appointed full professor in 2013.

THE FUNDAMENTALS OF LIGHT IN PHOTONICS

The previously described effects and applications of photonics are based on the fact that light is an electromagnetic wave. The fundamental idea can be illustrated using a familiar form of waves, such as water waves. From those we can see that a wave oscillates in time while traveling through space. But where a water wave requires liquid as medium, electromagnetic waves travel freely through space – instead of the medium, the electric and magnetic fields oscillate. A key quantifier of waves is wavelength, which measures the distance from one wave maximum to the next (see Figure 1a). For water waves, the wavelength ranges from centimeters to few hundreds of meters. Electromagnetic waves also exist at these wavelengths – those are the radio waves as known from radio/tv broadcasting, radar, Wi-Fi or mobile phones. But only if the wavelength of electromagnetic waves is much smaller – about one-millionth of a meter – they trigger signals in the receptors of the human retina, which enables us to see, and are known as visible light.

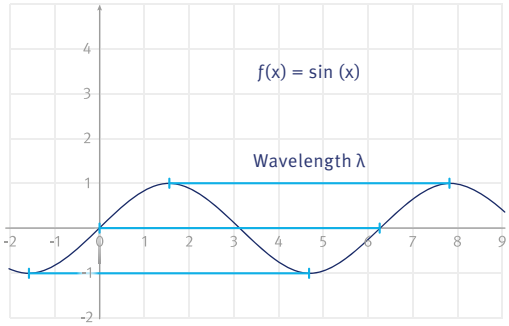


Fig. 1a

Exactly as water waves scatter and reflect off stones, bridges, and shores, in photonics one can utilize different materials to scatter and

Dr. André Hildebrandt

André Hildebrandt recently completed his PhD in the Prof. Förstner's research group in the area of "Micro- and Nanostructures in Optoelectronics & Photonics". His research focus is on applied and integrated Optics and Numerics. Previously, he has been working for the automotive company Hella KG for several years after graduating from Paderborn University with his Master's thesis "Numerical Simulation of light coupling into photonic crystal defect wave guide".

reflect light waves. One interesting property is that waves coming from two directions can both constructively and deconstructively interfere with each other. While this interference is rarely exploited for water waves, it is often utilized in photonics to radiate light into a certain direction, to guide it onto a particular molecule, to focus it into a desired area, or to direct it towards an optical sensor.

To make optimal use of this interference effect, however, the structures must have features smaller than the optical wavelength i.e., the range of few nanometers – used today in modern lithography equipment such as that available in Paderborn's CeOPP center.

Additionally, the range of possibilities extends beyond the geometry and also to the type of material that can be varied. For example, for some materials light travels faster than in others, and in the case of metals, light sticks to the surface and is partially converted to heat. And in so-called nonlinear materials, the oscillation frequency, and with it, the color of the light can be converted – which is quite handy if one only has a red light diode but needs green light.

All these effects, ranging from the interference of electromagnetic waves to material properties, are mapped to problem-specific models addressed by the group of Jens Förstner using physical equations. The variety of materials and geometries within one simulation leads to large and complex systems of equations requiring numerical evaluation. For this, the structures and the surrounding space is decomposed into many small spatial elements, which are then stored and processed in a computer. But often many elements are necessary that cannot completely fit into the memory of a single computer. Here, PC² comes into play.

Our model is distributed onto dozens to hundreds of computers, each storing and computing only a small part of the full space. However, since light travels between these parts, the computers have to exchange the relevant infor-

Constructive interference

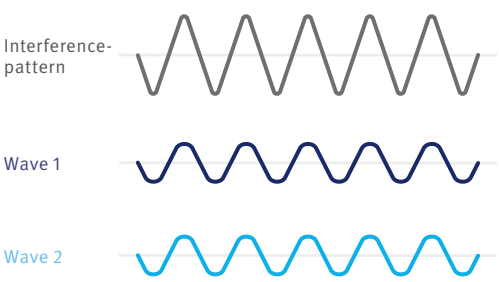


Fig. 1b

Destructive interference

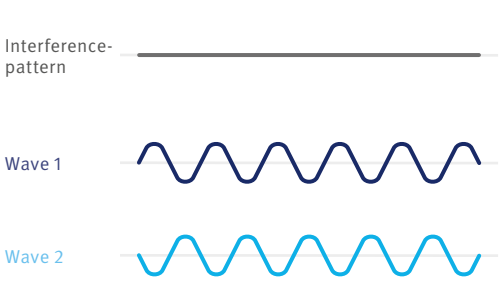


Fig. 1c

mation – and therein lies the strength of high-performance computing centers like the PC² with their special and fast network interfaces.

The figures show examples for structures investigated by Förstner's group. First, Fig. 2 illustrates a structure optimized to capture light from outside and to focus it into a small area (i.e., on the order of an embedded molecule). To achieve the best possible light concentration over 1,000 different models with a systematic variation of parameters, were simulated on the PC² computer cluster. The shown geometry performs several times better compared to existing solutions.

The structure in Fig. 3 represents an optical antenna – a miniaturization of a radio-frequency roof antenna to the nanoscale making it suitable for optical light. By using simulations on the PC² cluster it was possible to show that the proposed structure has a better directional characteristic compared to existing optical antennas. Although the calculations have only recently been finalized, there are already experimental results from co-workers which confirm the efficiency of the design.

With this work, a wide spectrum of other photonic structures has been investigated by Förstner's group including metamaterials, photonic crystals, quantum dots, integrated waveguides, biological structures – and even interplanetary dust.

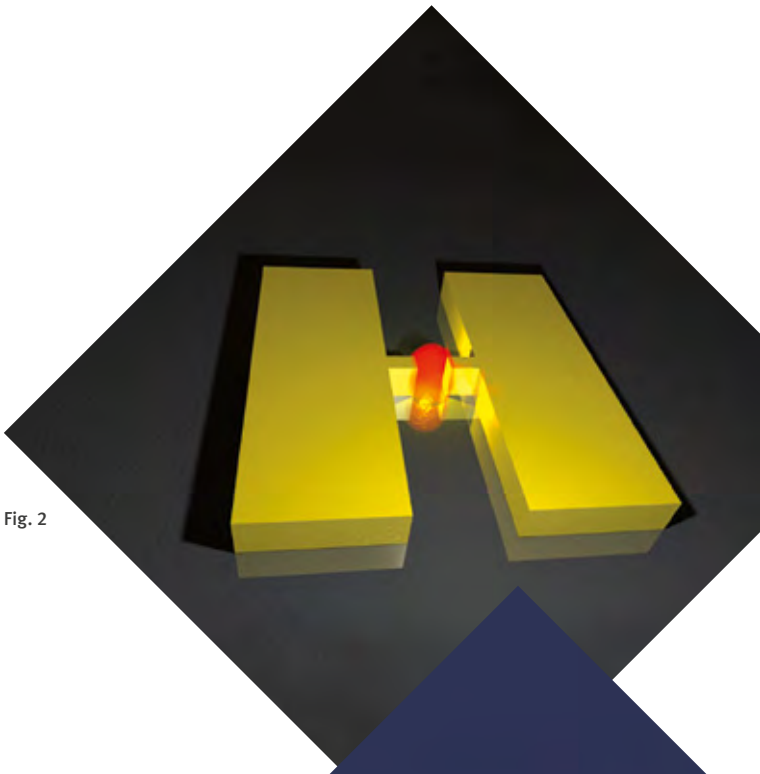


Fig. 2

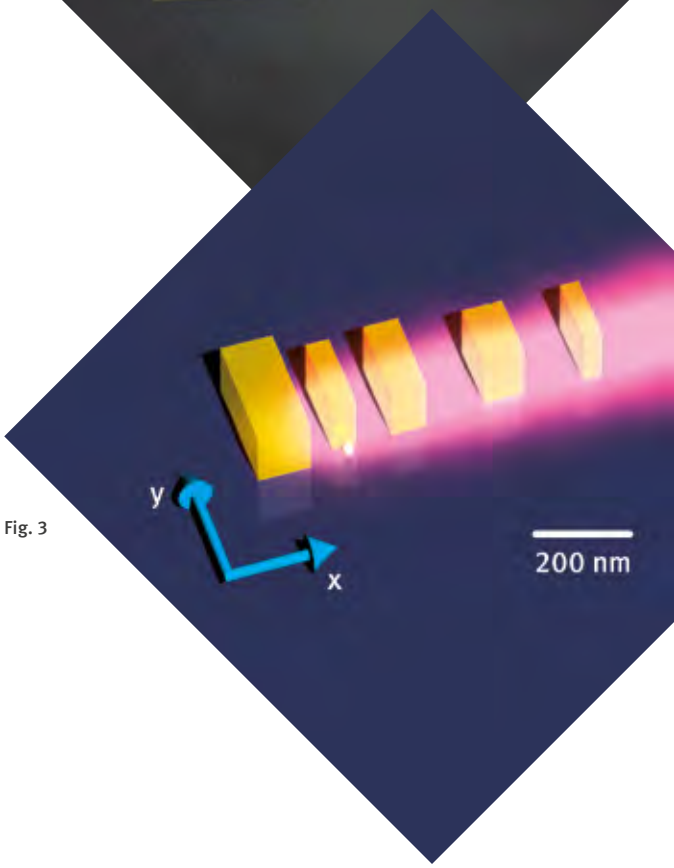


Fig. 3


ADVANCED ALGORITHMS MEET HIGH-PERFORMANCE COMPUTING, FOR A GAME OF GO

Games are an excellent way to test new ideas in artificial intelligence; they provide a clear environment for experimenting with strategies and allow for a direct comparison to humans. The Chinese board game Go is particularly interesting because of the sheer number of possible moves, which requires players to often rely on intuition. Previously, computers were considered inferior to humans, although that was challenged early last year when a program by Google DeepMind called AlphaGo won a match against the world's top champion.

At Paderborn University, research in computer Go started in 2006 with a student project group to design a parallel program distributed onto a computer cluster accelerated by FPGAs. In cooperation with Microsoft Research, Dr. Lars Schäfers continued this work and went on to create Gomorra. Gomorra ran on up to 2,048 cores on the OCuLUS cluster of PC². Our current flagship Go program is called Abakus, developed by Tobias Graf.

The dominant algorithm in computer Go is Monte Carlo Tree Search. Starting from the current board position, Abakus investigates possible continuations of the game through tree search and evaluates the resulting positions by randomly playing moves until the game ends, building statistics about win rates along the way. Then the calculated move with the highest winrate is played. To reduce the search space (i.e. the number of available moves), Abakus uses advanced techniques like deep convolutional neural networks, which give advice on the relevance of each move.

Currently, Abakus is ranked as strong "6-dan" player running on 12 nodes of the OCuLUS cluster with 192 CPU cores and 12 Tesla GPU cards accelerating the deep convolutional neural networks. At the Computer Olympiad in 2016, Abakus won two gold medals and one silver medal, making it one of the world's best Go programs.

Prof. Dr. Marco Platzner

Marco Platzner heads the Computer Engineering group at Paderborn University. Previously, he held researcher positions at ETH Zurich, Stanford University, the GMD – Research Center for Information Technology, and the Graz University of Technology. He holds diploma and PhD degrees in Telematics (Graz University of Technology, 1991 and 1996), and a "Habilitation" degree for the area hardware-software codesign (ETH Zurich, 2002). His research interests include reconfigurable computing, hardware-software co-design and parallel architectures.


QUANTUM
EFFECTS IN
CHEMICAL
REACTIONS

1st PRINCIPLE-BASED SIMULATIONS FOR THE REACTION OF METHANE WITH ATOMS

In the quest to better understand chemical reactions, quantum dynamic simulations have revealed detailed insights, but the effects of energy-transfer between different motions of the reaction still raise questions: What influence has the vibrational and rotational energy of the reactants on the reaction probability? And will this affect the vibrational and rotational energy distribution of the products? These questions can today routinely be answered for triatomic reactions, but quantum mechanical simulations of polyatomic reactions remain difficult. Our group is researching the frontier of this area by looking at reactions of hydrogen, fluorine, and chlorine with methane.

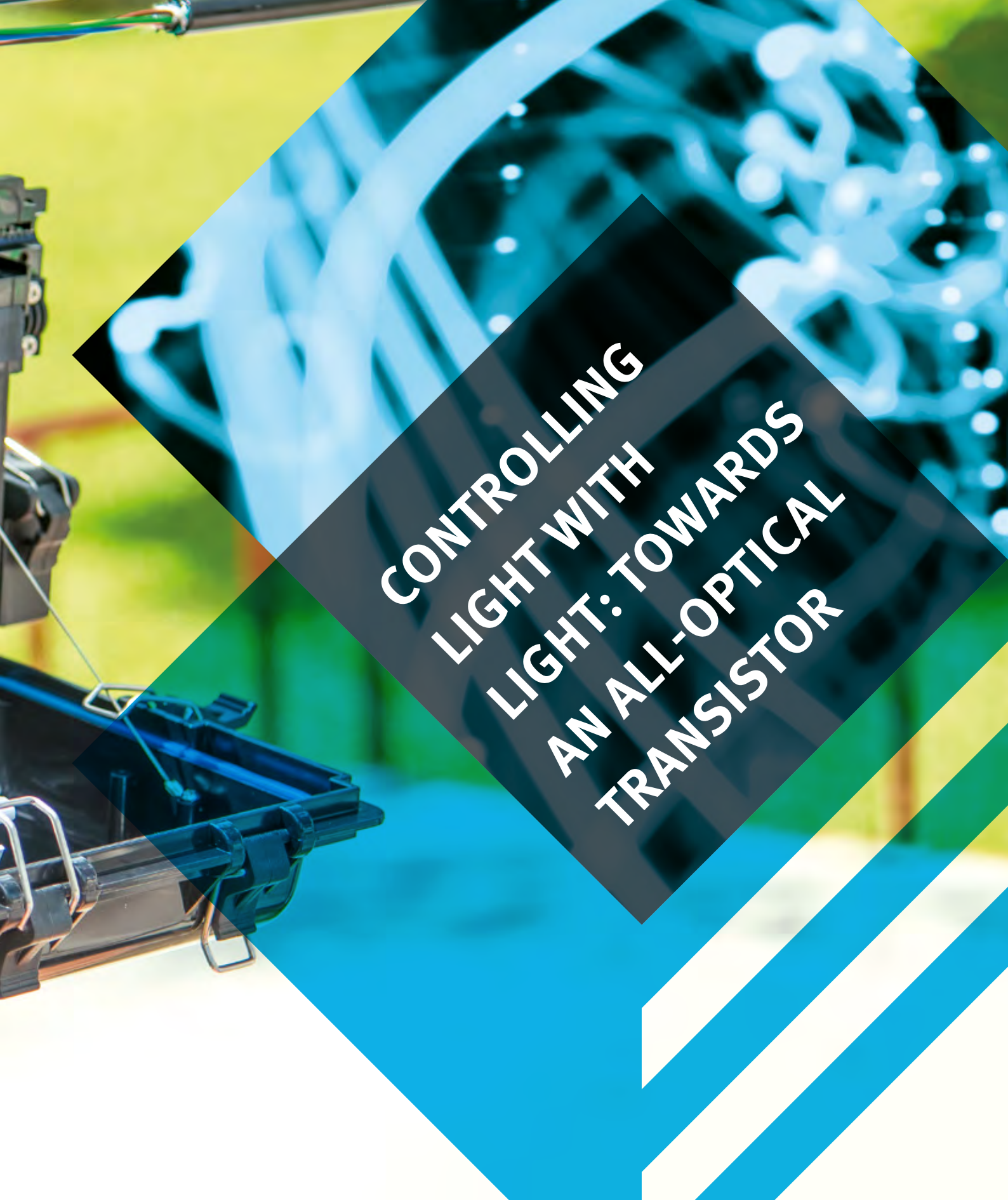
We have developed theoretical and numerical methods to address this problem through a specific algorithm used to solve very high-dimensional systems of differential equations. Known as the MCTDH approach, it can be used to describe molecular systems. Currently, we simulate diverse quantum effects in molecular systems, e.g., intramolecular proton transfer and quantum fluxuality in the CH_5^+ molecule; energy transfer effects between vibrational and rotational modes of reactants in the reaction of hydrogen with methane and its isotopic analogues; or resonances in the entrance channel of the $F+CH_4$ reaction. The PC² HPC systems are ideally suited to perform parallelized computations with our MCTDH and investigate these quantum effects that are observed in impressive experiments.

Prof. Dr. Uwe Manthe

Uwe Manthe has been professor for Theoretical Chemistry at Bielefeld University since 2004. His primary research interests are quantum effects in chemical reaction dynamics. Additionally, he works on the development of efficient numerical methods for quantum molecular dynamics simulations, which requires solving extremely high-dimensional differential equations.

M.Sc. Roman Ellerbrock

Roman Ellerbrock has been working on his PhD in Prof. Dr. Uwe Manthe's group since graduating from Bielefeld University in 2014. His research is focused on developing the fundamental theory of reaction dynamics and describing the reaction of atoms with methane through quantum dynamics simulations.



CONTROLLING LIGHT WITH LIGHT: TOWARDS AN ALL-OPTICAL TRANSISTOR

Light is ideally suited for long-distance data transmission. However, signal processing in nodes of communication networks typically requires optical signals to be converted into electrical signals and then re-converted into optical signals for further transmission. Processing operations such as reading, targeted forwarding, and re-direction of data can be easily implemented in electronic circuits. However, a purely optical approach would eliminate the necessity to convert into electrical signals.

A key element in optical circuits is an optical switch. Its characteristic feature is that a light signal is changed or switched by another light signal, such as in its amplitude, its direction of propagation, or its polarization state. However, light waves do not interact directly (by principle of superposition) such that any active manipulation can only be achieved in nonlinear optical media. Unfortunately, optical nonlinearities are mostly intrinsically weak. As a consequence, relevant signal changes can often only be achieved with strong control fields that undermine the idea of cascadability, wherein the switched signal itself can be used to trigger another switching operation. Also, the increasing demand for miniaturization calls for optical components operating at low light intensities. One approach to enable optical switching at very low light intensities is based on optical patterns [1, 2]. Besides switching at absolutely low intensities, in this approach, transistor-like responses can be achieved where a weak optical beam controls a stronger one, a pre-requisite for cascadability [2, 3].

The present work is based on a specific nonlinear phenomenon called self-organization, which is ubiquitous in nature. Prominent examples are spontaneously formed regular spatial structures for example in water-flooded sand, animal coat patterns, or geographical variations in the population of parasitic insects [1]. In all these examples, as a result of nonlinearity, certain observables do not reflect the symmetry of the actual system, i.e., spatial homogeneity. The microscopic origins of the underlying non-

Prof. Dr. Stefan Schumacher

Stefan Schumacher is head of the Theory of Functional Photonic Structures group at Paderborn University. Previously he held appointments at University of Arizona, USA, Heriot-Watt University in Edinburgh, UK, and Universität Bremen. His research group studies the fundamental physics of linear and nonlinear optical properties of semiconductor and molecular nanostructures for future applications in optoelectronics and photonics.

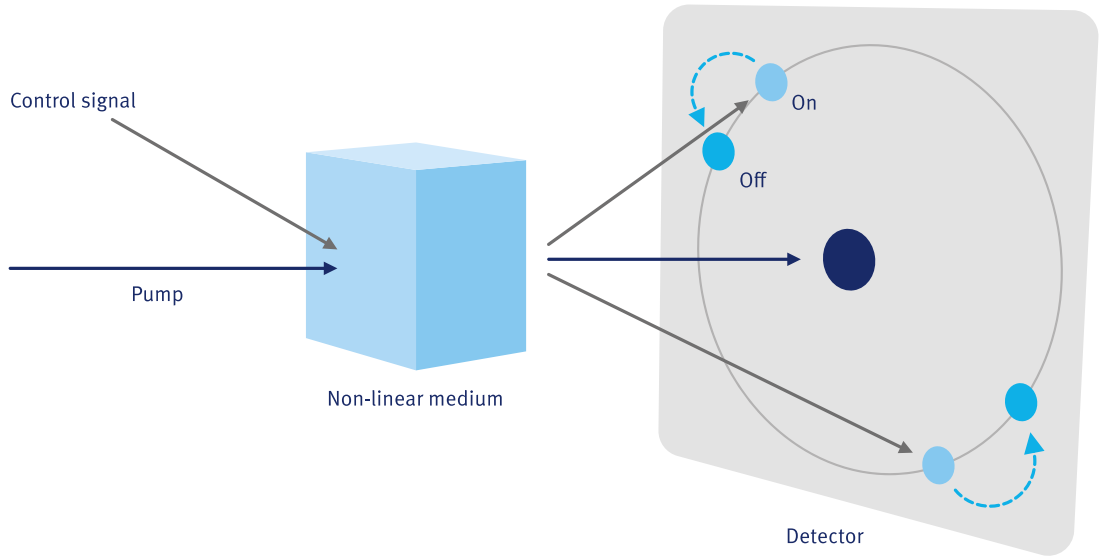


Fig. 1: Simplified illustration of a switching process based on optical patterns in a non-linear medium. The figure shows the ON state. When the control signal is switched off, the system and the detected signal revert to the OFF state.

linearities are as diverse as the phenomena themselves. In general, observables in linear systems change in proportion to an excitation or driving force. This may be fundamentally different in nonlinear systems. The behavior of a nonlinear system can depend drastically on excitation intensity so that the system behavior does not change continuously but rather drastically when a critical excitation intensity is reached.

In the present work, optically induced abrupt transitions between stationary optical patterns in a nonlinear medium are used for optical switching (Figure 1). A spontaneously formed pattern is used as the initial state or starting point for the switch. The formation of a spatial optical pattern inside the medium (not shown in Figure 1) translates into directed emission of light from the system. The switching action is then triggered by a weak control pulse/beam that steers the emitted light into another spatial direction. The switched signals revert back to their initial direction when the control pulse is switched off. The basic switching principle, where the ON and OFF states of the switch are encoded in different spatial orientations of the emission, is illustrated in Figure 1. To achieve favorable performance, the system is operated in a parameter range, where due to the nonlinearity, minor perturbations can result in abrupt changes of macroscopic behavior, in this case, emissions in different directions. It can be shown that this optical switching principle meets the essential requirement of cascadability, providing a transistor-like response where stronger optical signals are switched by weak optical controls [2, 3].

The principle discussed above was first demonstrated using a hot atomic vapor as a nonlinear medium [2]. A technologically more relevant way to implement the same principle is based on a compact semiconductor quantum-well microresonator. The fundamental physics behind the nonlinearities in the semiconductor system is totally different from the atomic system and is related to complicated many-body interactions and scattering among the quantum-mechanical particles [3]. However, the general principles of pattern formation and of the controlled and reversible transitions between the different states is transferable [3]. The experimental implementation in [4] required a tailored structure with two coupled optical resonators which can be fabricated using modern epitaxial crystal growth methods. The patterns preferentially formed in these systems are hexagons. These can be transformed into other patterns by modifying the optical excitation. For instance, slight tilting of the pump laser leads to instability of the hexagon so that only two spots are observed on the screen as in Figure 2. If an additional control beam is switched on, the signal is switched. From the computed system dynamics, we find that the switching can occur on a timescale of 100 picoseconds (one ten-thousandth of one millionth of a second [5]).

Pattern formation and its optical control in semiconductor microresonators relate to various fields of physics such as non-linear optics, non-linear dynamics as well as semiconductor and many-body physics. Not least due to this fact, this field holds much potential for exciting fundamental research. With regard to optical

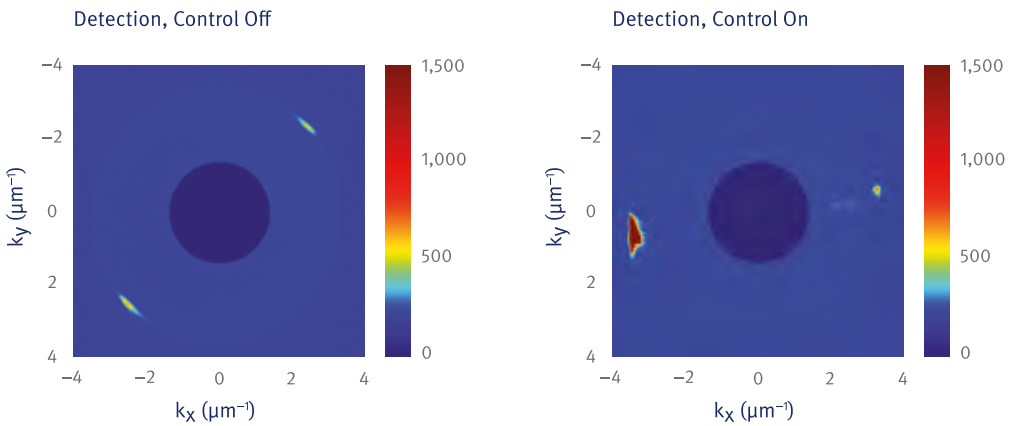
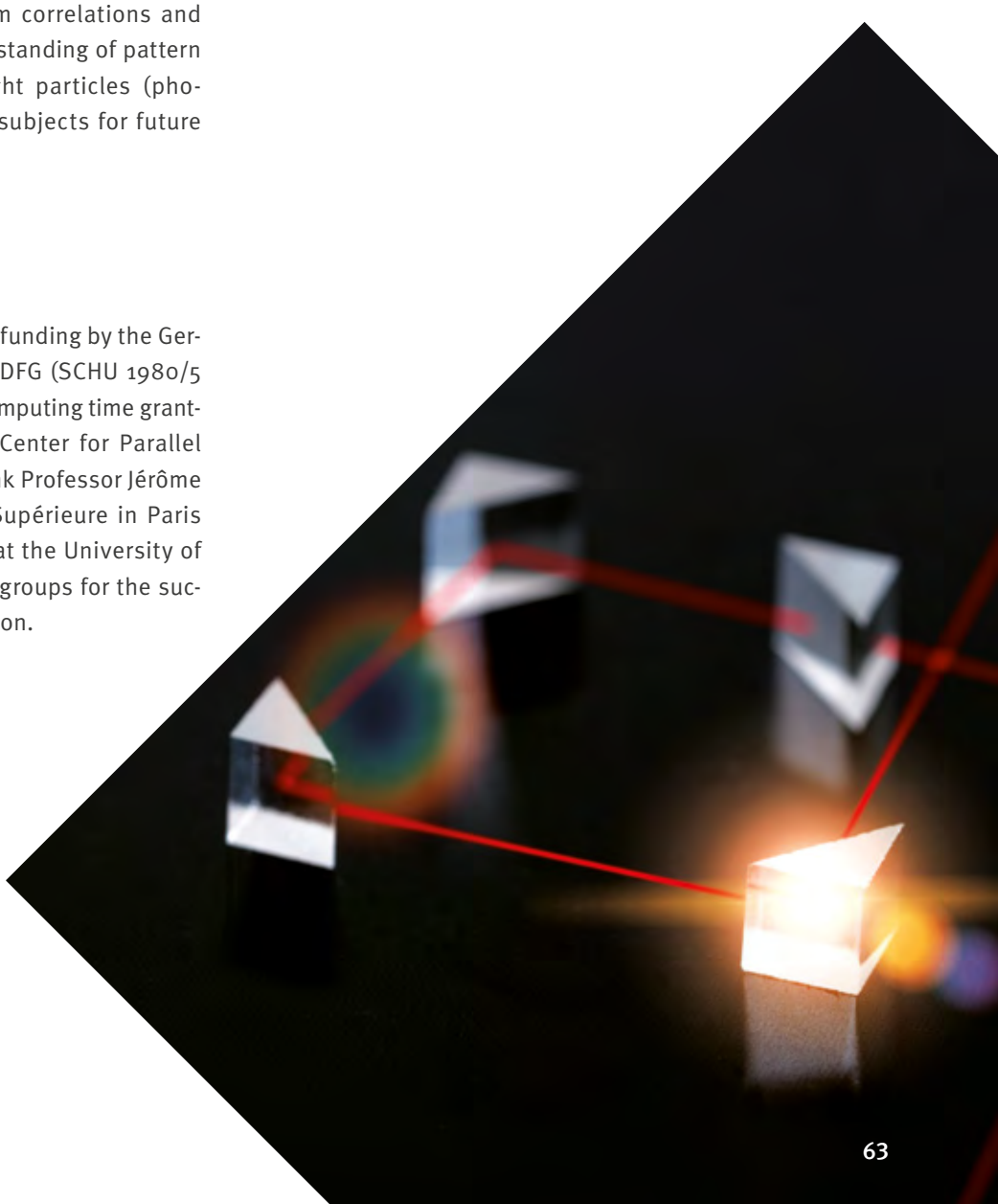


Fig. 2: Experiment on switching with patterns in a double-microresonator. Data from [4].

technologies, semiconductor materials with a large band gap such as gallium nitride and zinc oxide as well as organic molecular systems will play an important role in the future. Electrically pumped microresonators also open up entirely new possibilities. Quantum correlations and the quantum-optical understanding of pattern control using only few light particles (photons) are also fascinating subjects for future research.

ACKNOWLEDGEMENTS

We gratefully acknowledge funding by the German Research Foundation DFG (SCHU 1980/5 and GRK 1464) as well as computing time granted by the PC² Paderborn Center for Parallel Computing. We further thank Professor Jérôme Tignon at École Normale Supérieure in Paris and Professor Rolf Binder at the University of Arizona and their research groups for the successful long-term cooperation.




TRANSPORT
COEFFICIENTS
IN QCD

Just a few seconds after the Big Bang, the Universe was a hot and dense soup of quarks and gluons, and was close to the transition point when protons and neutrons would emerge. These elementary particles, constituting all matter we know today, arose from the soup and in the process, created the most perfect liquid known to science.

Using large accelerators such as the Large Hadron Collider (LHC) at CERN in Geneva, heavy lead nuclei are smashed into each other at nearly the speed of light. For a short time, a small lump of matter, the Quark Gluon Plasma (QGP), is created that is as hot and dense as the early Universe. Experimental studies reveal that the QGP can be described by formulae derived for liquids. While they are relativistic formulae, they are similar to the hydrodynamic laws which govern things like the flow of water. But in order to fit the experimental results, the lowest viscosity ever measured must be assumed.

The quantum field theory for strong interactions involving quarks and gluons is known as Quantum Chromo Dynamics (QCD). With pencil and paper alone, it is not possible to compute from

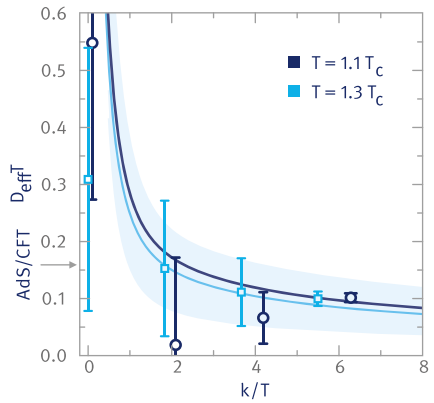


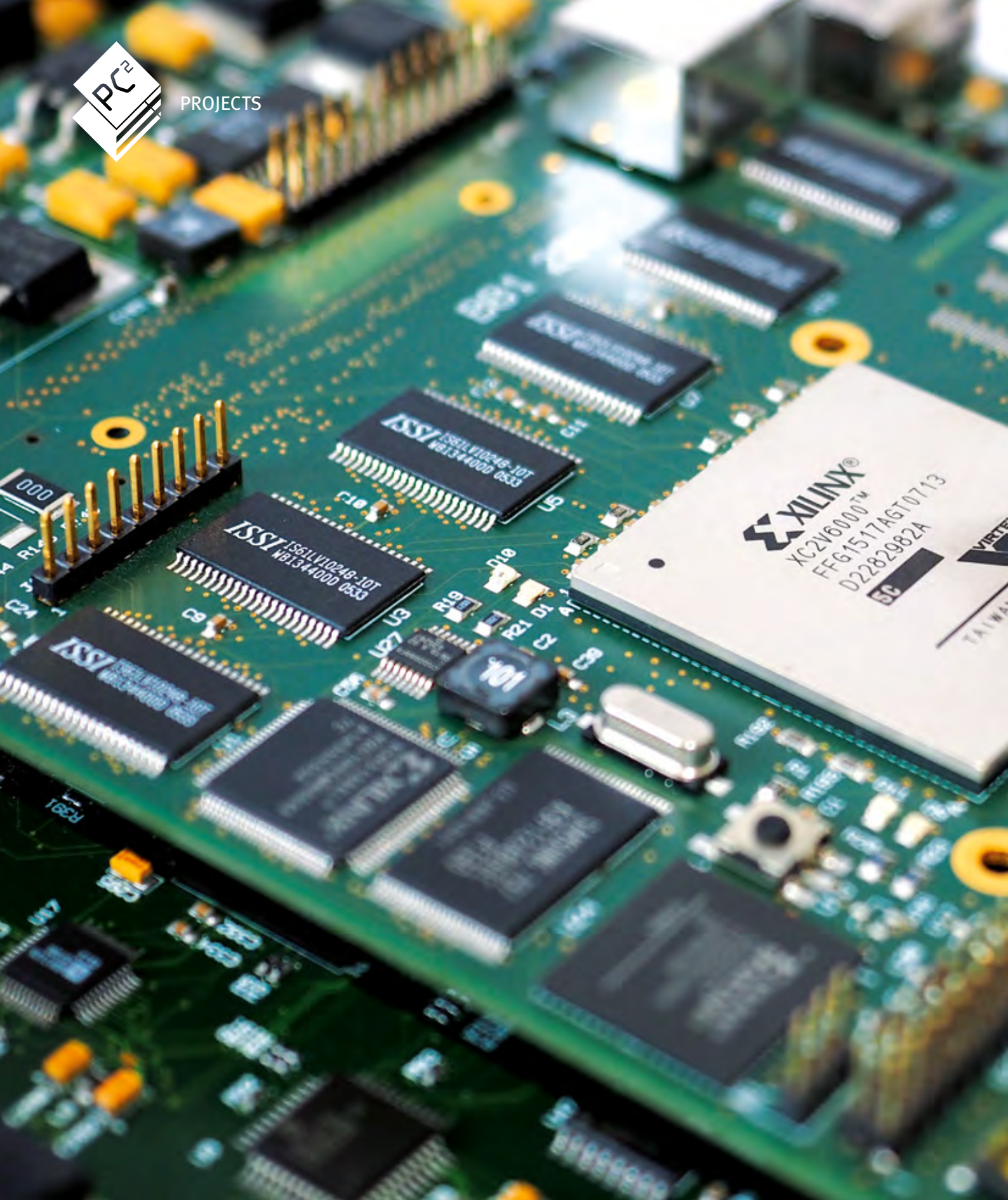
Fig. 1: Lattice QCD results of the momentum dependent coefficient Deff compared to a perturbative prediction.

QCD the behavior of a system of quarks and gluons in relevant temperature and density ranges. Instead, numerical techniques have to be applied, calling for HPC resources available at PC².

These studies require the computation of (noisy) correlation functions and the extraction of spectral information. As an example, in Fig. 1 we show a (momentum k dependent) diffusion coefficient D_{eff} at two different temperatures T [1] which in the limit of vanishing momentum is related to the electrical conductivity of the QGP. Obtaining a result like this requires fine-grained and large lattices.

Dr. Olaf Kaczmarek

Olaf Kaczmarek is a senior scientist at the University of Bielefeld where he also received his PhD in the year 2000. His research area is strongly interacting matter at high temperatures and densities using lattice discretized quantum field theory methods on high performance computers. His main interest is the determination of transport properties and in-medium modifications of hadrons in the Quark Gluon Plasma.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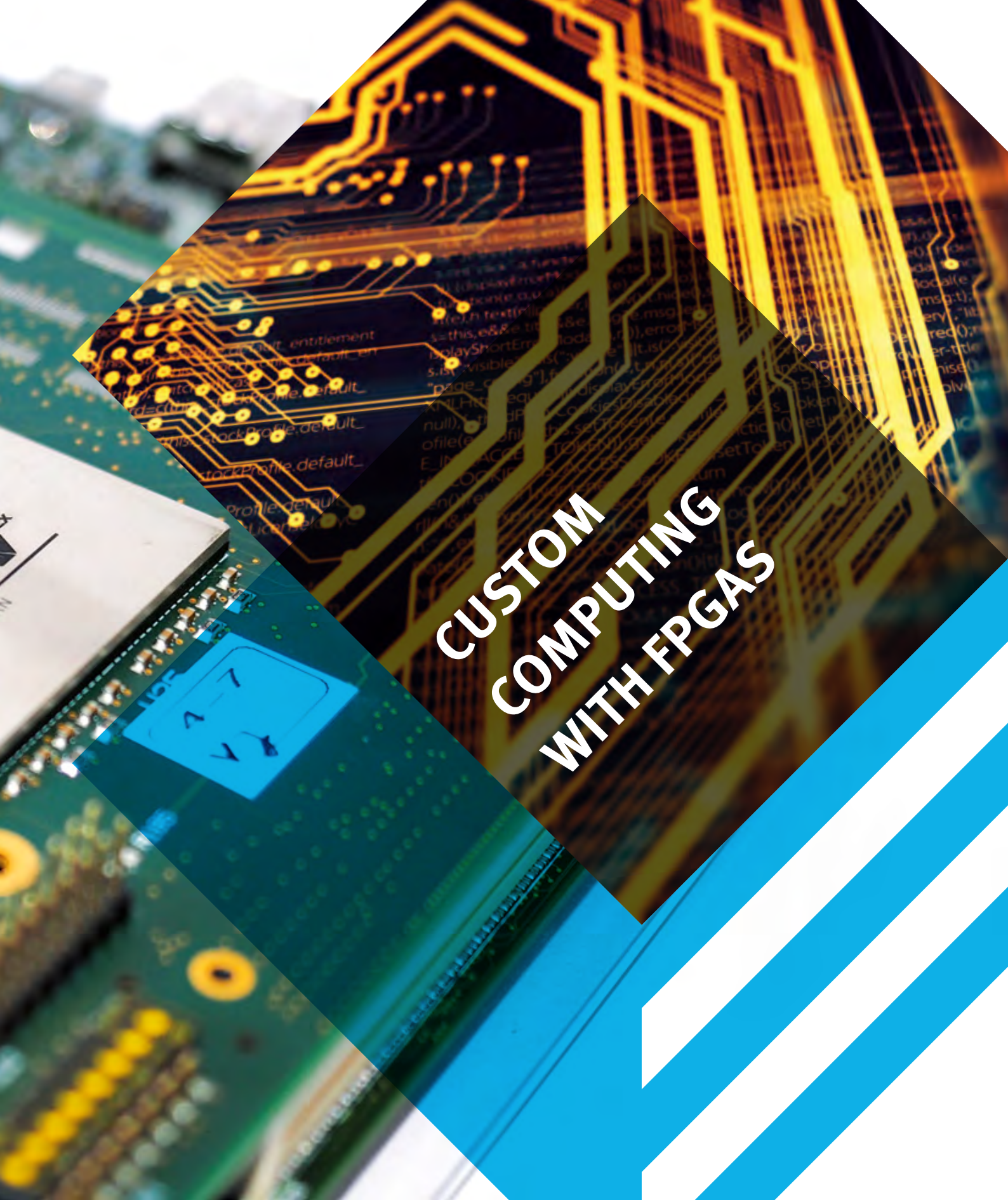

CUSTOM
COMPUTING
WITH FPGAS

WHAT IS AN FPGA?

Field-Programmable Gate Arrays (FPGAs) are reprogrammable electronic devices that comprise a very large number of basic electronic circuit components and a connection network. The function of the components and the structure of the connections between the components can be changed within a few milliseconds by downloading configuration data to the device. Thanks to the capability of FPGAs to implement any electronic circuit, they are the device of choice for applications that have demanding performance and energy consumption constraints that cannot be met by conventional processors and for which the development of a fixed-function silicon chip is too expensive or inflexible. FPGAs are widely used in telecommunications, networking and cryptographic applications. Beyond these mainstream applications, FPGAs have been used for the implementation of application-specific accelerators for many computationally challenging problems which is denoted as reconfigurable or custom computing.

Prof. Dr. Christian Plessl

Christian Plessl is professor for High-Performance IT Systems at the department of Computer Science at Paderborn University and the director of the Paderborn Center for Parallel Computing. He earned a PhD degree in Computer Engineering in 2006, and a MSc degree in Electrical Engineering in 2001, both from ETH Zurich. His research interests include architecture and tools for high-performance parallel and reconfigurable computing, hardware-software co-design, and adaptive computing systems.

INTERVIEW

Custom computing is a main pillar of PC²'s research and Patrizia Höfer met with Professor Christian Plessl and Dr. Tobias Kenter to discuss activities of PC² in this area.

PH: WHAT IS THE SIGNIFICANCE OF COMPUTER SIMULATION FOR SCIENCE AND ENGINEERING?

CP: Computer simulation has become increasingly important for many areas of science and engineering. Many physical phenomena can be well described at the microscopic level from first order principles. Based on these models, the dynamic behavior or steady-state of large scale systems can be simulated with high accuracy. The trend towards computational modeling is spreading rapidly to different domains including physics, chemistry and material science. Computer simulation and analysis are also expanding into domains which thus far have hardly been touched by these methods, such as economics, social sciences and even humanities.

PH: WHAT CHALLENGES DOES THIS POSE FOR PC²?

TK: I see two major challenges in this context. On the one hand, the desire to simulate increasingly complex problems raises the quantitative demand for computing resources at our center. Hence, we need larger computer systems. This brings additional challenges for power supply and cooling. On the other hand, the influx of new classes of users requires flexibility. Flexibility of the PC² staff, to understand user requirements and provide the right form of support. And the flexibility of the computing systems itself, to efficiently execute the upcoming workloads.

Dr. Tobias Kenter

Tobias Kenter is postdoctoral researcher in the High-Performance IT Systems group at Paderborn University and in the Paderborn Center for Parallel Computing. He completed his PhD at Paderborn University in 2016 and holds a Computer Science diploma from the same university. His research interests include methods for productive usage of FPGAs via high-level-synthesis or overlays, tradeoffs between specialization and generality of designs, and scalability of parallel systems with reconfigurable accelerators.

PH: HOW IS PC² ADDRESSING THESE CHALLENGES?

CP: We are currently planning the procurement of a new cluster system with latest-generation hardware and modern cooling concepts. A large part of this system will focus on standard processors that can best cover the diverse demands. But we also put extra emphasis on a particularly innovative and efficient accelerator architecture, FPGAs. The performance and energy efficiency potential of FPGAs has been demonstrated with prototypes in foundation-oriented research projects. But we strive to be at the forefront of introducing FPGAs production systems and – more importantly – production codes for high-performance computing.

When it comes to supporting users to make best use of these systems, PC² already has a good tradition of working with a mix of diverse users, including some users who don't originate from computational sciences. But of course, when it comes to making the best use of FPGA accelerators, we need to expand our support in that area. This is where Tobias' and my background in custom and reconfigurable computing come into play.

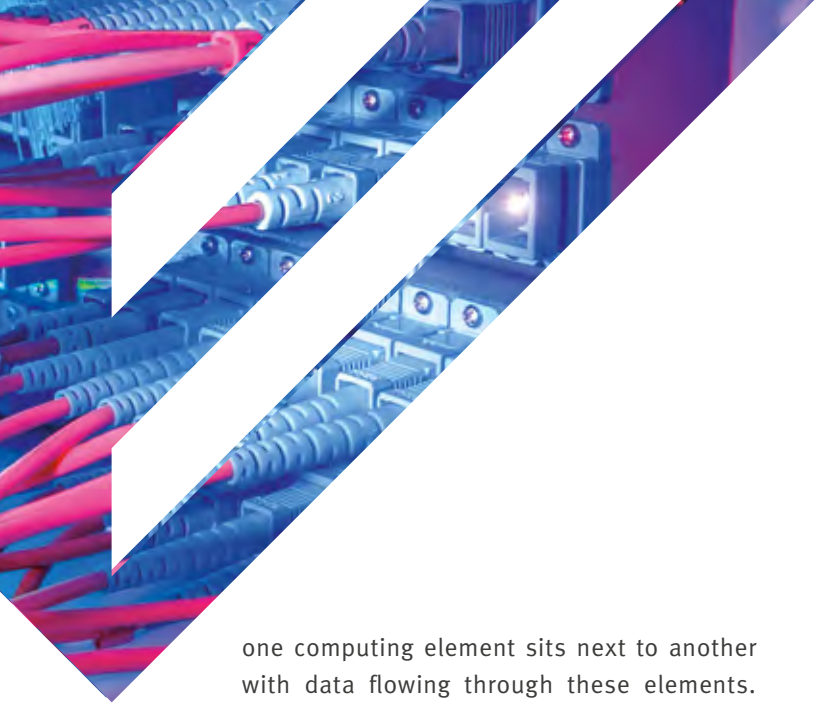
PH: WHAT IS THIS RESEARCH ABOUT?

CP: Since the very early days of FPGAs more than 25 years ago, the so-called reconfigurable computing community has explored ways to use architectures like FPGAs to perform computing tasks that would traditionally run on processors. Custom Computing leverages this approach, but adds an additional focus to the interplay between applications and architectures, and also deliberate use of system heterogeneity. For example, in the recently finished EU-funded project SAVE, we contributed a runtime system for transparent workload migration to heterogeneous resources and just-in-time code generation for GPUs and FPGAs.

TK: In the DFG-funded Collaborative Research Center On-The-Fly-Computing, we are working on similar challenges and put a special emphasis on reusable and configurable FPGA designs that are called overlays. Such overlays have huge advantages when the migration to an accelerator needs to happen quickly and mostly automatically. In a more classical HPC context, like our recent work on nanophotonics simulations on FPGAs, we pursue more time-consuming optimizations in order to reach the highest performance.

PH: BUT IF RECONFIGURABLE COMPUTING WITH FPGAS HAS ALREADY BEEN RESEARCHED THAT LONG, WHY WOULD IT SUDDENLY BE SUITABLE TO BE DEPLOYED IN A SCIENTIFIC COMPUTING CENTER WITH ITS FOCUS ON HIGHEST PERFORMANCE FOR DIFFERENT USERS?

TK: On a very basic computer architecture level, one could say that processors compute in time, that is, one step after the other. In contrast, FPGAs are computing in space, meaning



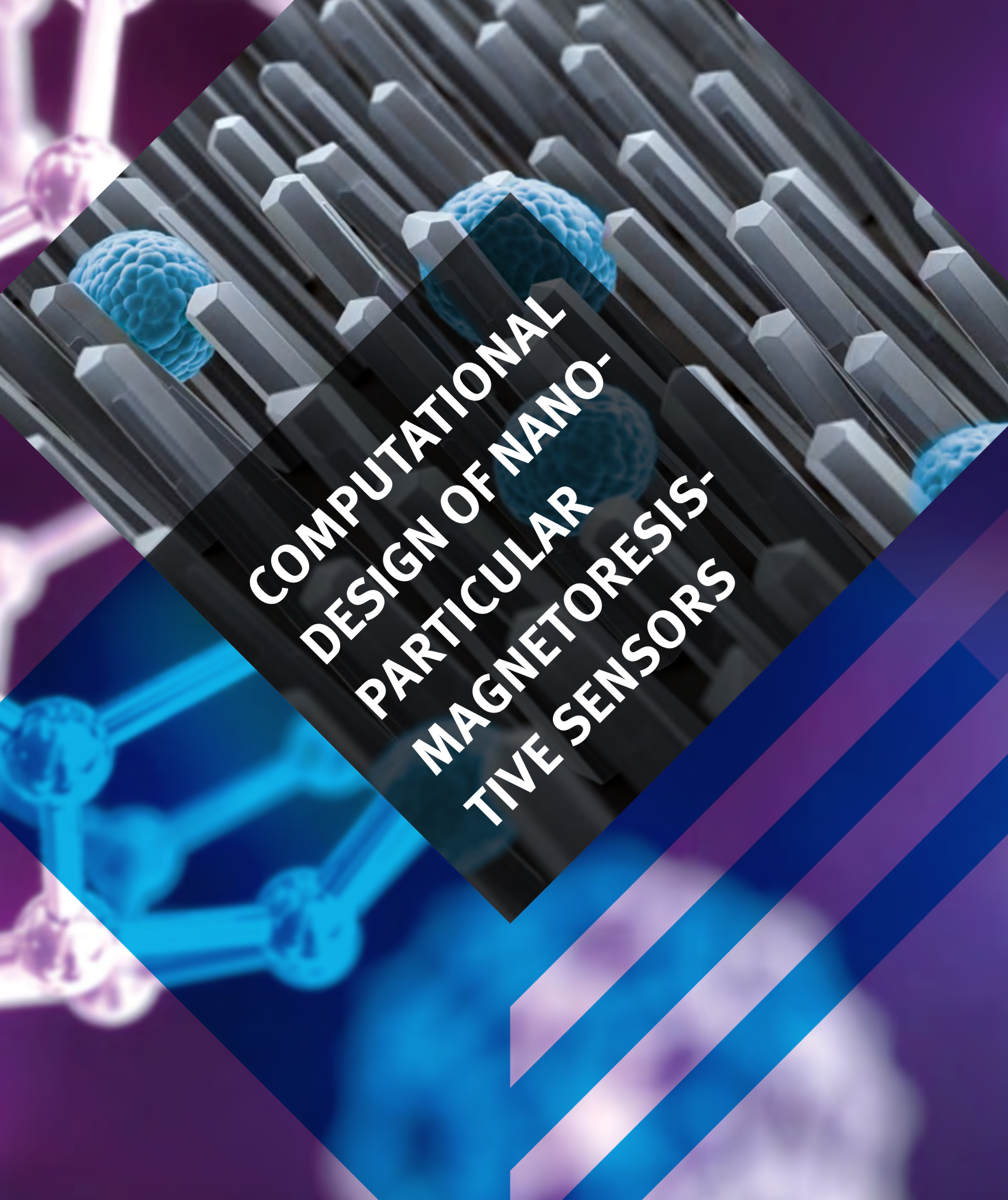
one computing element sits next to another with data flowing through these elements. Now, as technological advances have enabled manufacturers to fit more and more transistors on a single chip, the concept of computing in space arose naturally from the additional transistors. For processors on the other hand, it is becoming increasingly difficult to translate more transistors into faster or bigger sequential steps. Thus, over time FPGAs were able to catch up in achievable performance and even challenge CPUs on their home turf, which is floating-point intensive computations.

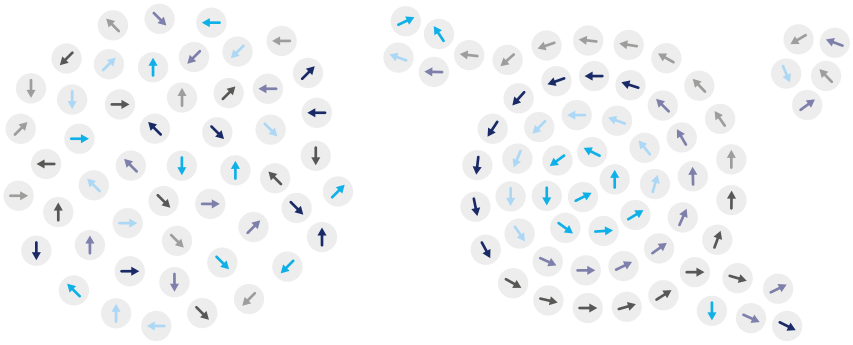
But there is much more to the current trend towards FPGAs. The design tools have improved a lot. We have reached a point were FPGA designs generated from high-level languages like C/C++ or OpenCL are actually usable. In the last two years, we have also seen the first generation of large-scale commercial FPGA installations at hyperscale cloud data-centers, e.g., from Microsoft, Baidu and Amazon. As a result, mainstream HPC technology providers like Intel or IBM are driving standardization of the software and hardware interfaces for integrating FPGAs in HPC systems. These new developments leverage FPGAs from a promising niche technology to a maturity that competes head to head with CPUs and GPUs.

PH: WHAT ARE THE NEXT STEPS YOU WILL TAKE WITH FPGAS AT PC²?

CP: We are currently starting two projects to boost the practical FPGA usage in scientific computing. In the DFG-funded project PerficienCC, we will work with users from Paderborn to find acceleration potential in their application codes. We will jointly develop FPGA designs for the most promising codes and spread their usage and further development through libraries and teaching materials. In the BMBF-funded project HighPerMeshes, a cooperation with three partner sites, we start at a higher abstraction and will build a comprehensive language and compiler framework for the specific application domain of simulations on unstructured meshes. FPGAs will be one target architecture for this framework, but we also aim for massive scaling over many compute nodes.

TK: Application scaling over many FPGA nodes is a topic that has hardly been touched by the reconfigurable computing community so far. With access to first cluster systems with FPGAs and with relevant applications, we hope to make a big impact with this topic at the intersection between reconfigurable computing and traditional HPC. We plan to further our position as a competence center in custom computing and to leverage our FPGA-enabled codes and our infrastructure to provide empirical results on the feasibility and benefits of custom computing.


COMPUTATIONAL
DESIGN OF NANO-
PARTICULAR
MAGNETORESIS-
TIVE SENSORS



Magnetoresistence (GMR) is a physical effect where electric properties of a material such as resistivity, is changed when a magnetic field acts on the material. Magnetoresistance, for example, is used in applications of biosensors which work by quantifying biomolecule coverage rates on sensor surfaces which is determined by a change in magnetoresistivity.

The formation of magnetic beads or nanoparticle superstructures, due to dipolar magnetic interactions, can be used to configure nanoparticular magnetoresistive sensors. It has been shown [1] that in systems of commercially available cobalt nanoparticles and novel silica [2] or agarose gels, large magnetoresistance amplitudes can be observed, making it a candidate for printable low-cost sensors [3].

By combining molecular dynamics and stochastic spin dynamics, we created a design tool that identifies potential beads or nanoparticle arrangements that result in high GMR-effects with high sensitivities. This enables us to study not only the static magnetic microstructure but also the dynamics of the structuring process itself in a gel matrix. The group utilized OCuLUS' CPU and GPU capabilities in a hybrid MPI and OpenMP approach for time-consuming calculations.

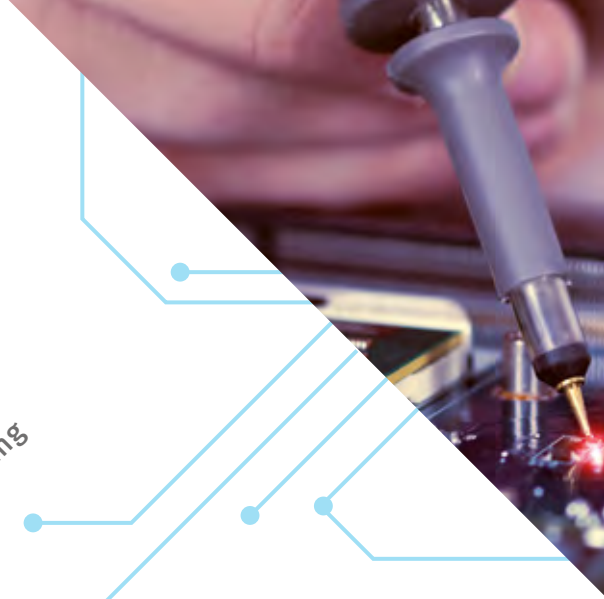
Prof. Dr. Christian Schröder

Christian Schröder received his PhD in theoretical physics in 1999. After working for Philips Research, Telelogic AB, and Ames Laboratory he became a professor at Bielefeld University of Applied Sciences in 2003. Schröder currently focuses on the theoretical modeling and numerical investigation of functional magnetic nanosystems, as well as high-performance computing and distributed computing methods.

TEACHING

LECTURES HELD BY MEMBERS OF PC²

In order to train students and PhD-level researchers in the effective use of computational methods for science, member of PC² and their working groups offer numerous courses, seminars and project groups in the domains of applied mathematics, computational science and computer science. The following overview shows a selection of our recent offerings.



COMPUTER SCIENCE

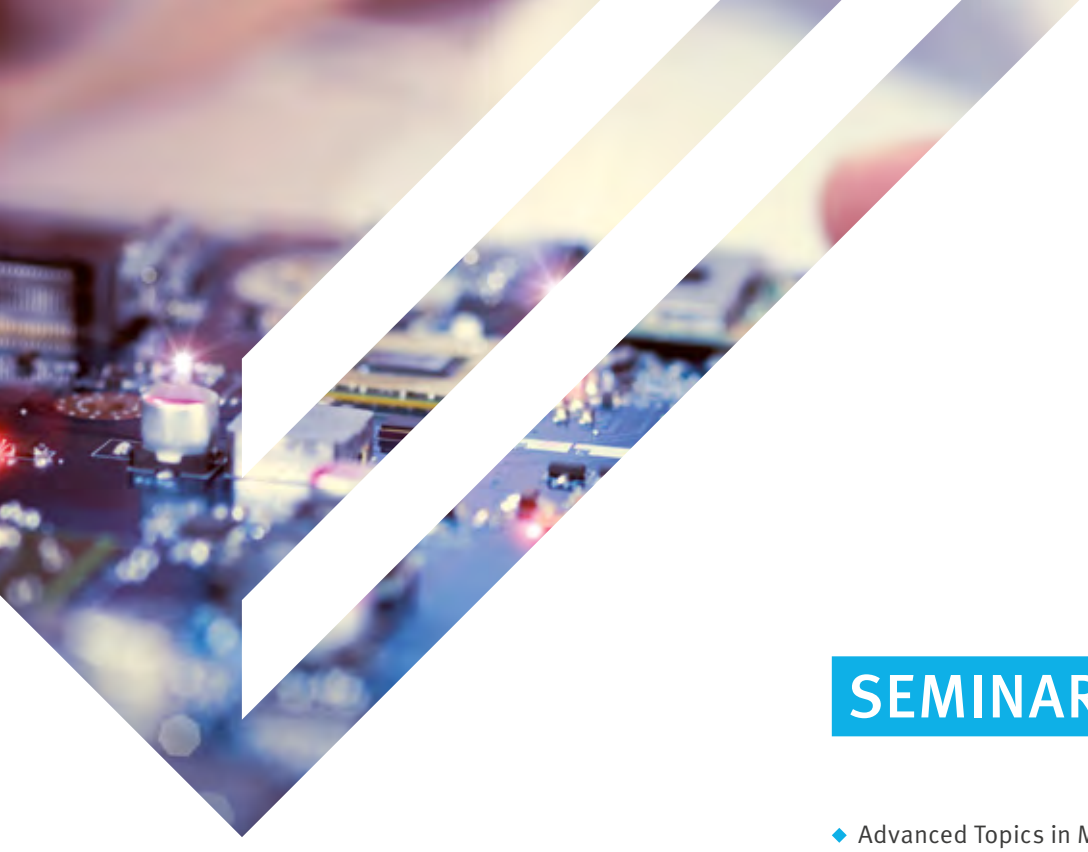
Distributed Systems | Parallel Computer Architecture
Advanced Computer Architecture | High-Performance Computing
Reconfigurable Computing

COMPUTATIONAL SCIENCE

Computer Physics | Quantum Chemistry
Theory of Functional Photonic Structures | Electromagnetic Field Simulations
Modeling and Simulation | Molecular Simulation

APPLIED MATHEMATICS

Numerical Simulations with the DG-TD Method
Algorithmic Differentiation | Numerics of Partial Differential Equations
Numerics | Computational Dynamics



SEMINARS

- Advanced Topics in Machine Learning
- Indexing and Searching Big Data
- Massively Parallel Computer Architectures
- Numerics
- Optoelectronics and Photonics
- Scientific Computing
- Unconventional and Approximate Computing

PROJECT GROUPS

- Approximate Computing
- Automatic Traffic Surveillance
- Customizing Neural Networks on FPGAs
- Distributed Cloud Functions
- Modeling and Simulation
- On-the-fly Computing for Big Data
- Practice of Electromagnetic Field Simulation

APPENDIX

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