HN FIZ Applied Quantum AI by Fraunhofer IAO & IPA

Fraunhofer HNFIZ

Fraunhofer Heilbronn Forschungs- und Innovationszentren HNFIZ

Symposium FTQC4NSc

Fault-Tolerant Quantum Computing for Natural Sciences

experimenta | Heilbronn
6th – 8th July 2026

ORGANIZED BY flaQship

IN COOPERATION WITH

HHN HEILBRONN UNIVERSITY OF APPLIED SCIENCES

CASUS CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

Preface

"And by golly it's a wonderful problem, because it doesn't look so easy." When Richard Feynman spoke those words about simulating nature on a quantum machine, he captured both the promise and the difficulty that still define our field today. More than four decades later, the simulation of quantum systems remains one of the most compelling candidates for genuine quantum advantage, and the path toward has come into sharper focus than ever before. It is this convergence of ambition and tractability that makes our gathering at experimenta in Heilbronn from 6 to 8 July 2026 for the symposium Fault-Tolerant Quantum Computing for Natural Sciences (FTQC4NSc) particularly timely.

The premise of this meeting is that the long-promised milestone, quantum computers outperforming classical methods on problems of real scientific and industrial relevance, will not arrive through algorithmic cleverness alone, nor through hardware advances in isolation. It demands both: efficient, application-oriented quantum algorithms developed hand in hand with fault-tolerant, error-corrected machines capable of running them. Materials science and quantum chemistry sit at the heart of this story, where the strongly correlated problems that defeat classical computation are most abundant, and where the disruptive potential of quantum simulation could ripple across entire industries.

FTQC4NSc is built deliberately around three intertwined threads: fault-tolerant quantum algorithms, quantum error correction, and quantum simulation for the natural sciences. Rather than treating these as separate communities, we have sought to unite them in the same room: decoder designers alongside algorithm developers, hardware architects alongside computational chemists, academic researchers alongside colleagues from industry. Across three days, an exceptional roster of invited speakers from leading universities, national research centers, and the companies building today's quantum hardware and software will share where the frontier now stands, and where it remains hard.

The abstracts collected in this booklet are the foundation of that exchange. Alongside the invited lectures, they include the contributed talks and posters submitted in response to our open call: work spanning quantum computing in chemistry and materials science, advances in quantum error correction and fault tolerance, and new algorithms for scientific computing. We are grateful to everyone who answered that call. The breadth and quality of the contributions are a reminder that this field is carried forward by a growing and increasingly interconnected community.

This symposium is organized by flaQship together with the Center for Advanced Systems Understanding (CASUS) and Heilbronn University of Applied Sciences (HHN). It is the 2026 edition of a series of symposia of the Fraunhofer Research and Innovation Center for Applied Quantum AI at Heilbronn, addressing the topics of the Kompetenzzentrum Quantencomputing Baden-Württemberg (KQCBW). With this series, we pursue three guiding aims: to foster the exchange of knowledge, to strengthen connections between researchers and practitioners, and to support the transfer of expertise into Baden-Württemberg and the rapidly developing quantum technology region around Heilbronn.

We are delighted to welcome you to experimenta, Germany's largest educational science center, and a fitting setting for a meeting devoted to understanding nature through computation. Our hope is that these days offer not only a survey of recent progress but the kind of conversations that move a hard and wonderful problem a little closer to being solved.

We wish you an inspiring and productive symposium.

The FTQC4NSc Scientific Committee

Prof. Dr. David Kreplin (HHN)
Dr. Werner Dobrautz (CASUS)
Dr. Vamshi Katukuri (Fraunhofer IAO)
Dr. Andreas Sturm (Fraunhofer IAO)
Dr. Jan Schnabel (Fraunhofer IPA)

List of Contents

Program

Day 1: Monday | July 6, 2026

08:45 **Opening**
Dr. Vamshi Mohan Katukuri und Dr. Marco Roth, Fraunhofer IAO / flaQship

09:00 **Invited Talk I**
Bringing quantum logic into quantum error correction | Prof. Jens Eisert, Freie Universität Berlin

09:45 **Invited Talk II**
Fast logic for the surface code: a challenge for decoding | Prof. Dr. Barbara M. Terhal, Delft University of Technology / QuTech

10:30 **Break**

11:00 **Invited Talk III**
Significantly more efficient Clifford+T synthesis for small-angle rotations and application to Trotterization | Dr. Nick Blunt, Riverlane Ltd.

11:45 **Contributed Talk I**
Polylogarithmic-Depth Quantum Algorithm for Simulating the Extended Hubbard Model on a Two-Dimensional Lattice Using the Fast Multipole Method | Yu Wang, Technical University of Munich

12:05 **Contributed Talk II**
Addressable fault-tolerant universal quantum gate operations for high-rate lift-connected surface codes | Dr. Sascha Heußen, neQxt

12:25 **Lunch Break**

13:55 **Invited Talk IV**
End-to-End Efficiency in Dissipative Preparation of Thermal and Ground States | Prof. Lin Lin, University of California, Berkeley / Caltech

14:40 **Invited Talk V**
Utility-scale electronic structure with under 100k physical qubits | Dr. Guang Hao Low, Google Quantum AI

15:25 **Break**

15:55 **Invited Talk VI**
Robust characterization of average gate set noise and cross-talk using gate-set shadows | Jadwiga Wilkens, Johannes Kepler University Linz

16:15 **Contributed Talk III**
Logarithmic-depth quantum state preparation of polynomials | César Feniou, Qubit Pharmaceuticals

18:30 **Conference Dinner**

Day 2: Tuesday | July 7, 2026

08:30 **Invited Talk VII**
Towards fault tolerant quantum computation on the Rydberg platform | Prof. Dr. Hans Peter Büchler, University of Stuttgart

09:15 **Invited Talk VIII**
Path to Starling – Realizing fault-tolerant quantum computation at scale | Dr. Tristan Müller, IBM Research Ehningen

10:00 **Contributed Talk IV**
Fast simulations of the Fermi-Hubbard model on the SPOQC architecture | Théo Dessertaine, Quandela

10:20 **Break**

10:50 **Invited Talk IX**
Leveraging low energy assumptions for quantum speedups | Dr. Nicholas Rubin, Google Quantum AI

11:35 **Contributed Talk V**
Reformulating Quantum Imaginary-Time Evolution via Curvature and Higher-Order Statistical Information | Dr. Carlos Benavides-Riveros, IQM Quantum Computers

11:55 **Contributed Talk VI**
Quantum Dynamics: The Next Frontier of Quantum Applications | Danial Motlagh, Xanadu Quantum Technologies

12:15 **Lunch Break**

13:45 **Invited Talk X**
Fitting quantum chemistry simulations of early fault tolerant quantum computers | Dr. Christian Gogolin, Covestro

14:30 **Invited Talk XI**
From Quantum Algorithms to Better Therapies and Materials: Transitioning from Near-Term to Early Fault-Tolerant Impact in Life Sciences and Materials Discovery | Dr. Stefan Knecht, Algorithmiq

15:15 **Break**

15:45 **Invited Talk XII**
Pauli and Majorana Propagation Methods for Supporting Chemistry and Materials Workflows on Quantum Hardware | Prof. Zoë Holmes, EPFL

16:30 **Invited Talk XIII**
Parallel Quantum Chemistry on NISQ Computers: From RDMFT Subsystems to Embedded Materials | Prof. Thomas Kühne, CASUS

17:15 **Contributed Talk VII**
Bypassing the Condition Number: Near-Optimal Quantum Solvers for Stationary PDEs | Matthias Deiml, University of Augsburg

18:00 **Poster Session**

Day 3: Wednesday | July 8, 2026

08:30 **Invited Talk XIV**
A framework for spin-adapted quantum chemistry on quantum computers | Dr. Nathan Fitzpatrick, Quantinuum

09:15 **Invited Talk XV**
One and Many-Body Aspects of Electronic Structure on Quantum Computers | Prof. Dr. Jakob Kottmann, University of Augsburg

10:00 **Contributed Talk VIII**
Rapid Dissipative Ground State Preparation at Chemical Transition States | Soumya Sarkar, University of Technology Sydney

10:20 **Break**

10:50 **Invited Talk XVI**
Spectroscopy use cases for fault-tolerant quantum computing | Dr. Jan Reiner, HQS Quantum Simulations

11:35 **Contributed Talk IX**
Simulating Electron Transfer on Noisy Quantum Computers | Marvin Gajewski, German Aerospace Center (DLR)

11:55 **Contributed Talk X**
Early fault-tolerant resource estimation for ground-state preparation via Lindblad simulation | Dr. Marius Bothe, Riverlane Ltd

12:15 **Lunch Break**

13:45 **Invited Talk XVII**
Near-term and fault-tolerant quantum computing applications in the natural sciences | Dr. Ivano Tavernelli, IBM Quantum

14:30 **Invited Talk XVIII**
Imaginary-time evolution in the age of quantum computing |
Dr. Fedor Šimkovic, IQM Quantum Computers

15:15 **Invited Talk XIX**
Scientific Challenges to Apply Quantum Computing in Drug Design |
Dr. Michael Streif, Boehringer Ingelheim

16:00 **Conclusion**

16:15 **End**

Invited Talks

Bringing quantum logic into quantum error correction | Prof. Jens Eisert, Freie Universität Berlin

Quantum computers promise computational advantages over classical supercomputers for certain tasks. However, this promise can only be realized if effective methods are employed to address the unavoidable errors present in practical implementations. While quantum error mitigation will continue to play an important role, it alone cannot enable scalable quantum computing [1]. Quantum error correction, by contrast, can detect and correct errors without revealing any logical information. Although the concept is not new, recent years have witnessed remarkable progress in the field. This advancement has been largely driven by substantial experimental breakthroughs, which in turn have accelerated theoretical developments. Today, quantum error correction is widely regarded as one of the fastest-growing subfields of quantum computing. This talk will guide you through several recent developments, with an emphasis on our own contributions to the field over the past two years [2–8]. We will explore the design of new Floquet codes [2, 3], accompanied by novel graphical calculi [2], and discuss detector error models [4].

At the heart of this talk lies one of the most actively discussed questions in the field today: how to perform practical quantum logic using quantum low-density parity-check (qLDPC) codes. While the mere existence of "good" such codes with highly attractive parameters has already marked a significant breakthrough, recent work has increasingly focused on how to realize fault-tolerant quantum computation with them in practice. The core part of the talk will present a particularly promising scheme that enables the compilation of fault-tolerant logical operations. To address the challenge that logical qubits do not necessarily map to disjoint sets of physical qubits, we introduce clustered-cyclic codes [5]—a family of quantum low-density parity-check codes with finite-size instances such as [[136,8,14]] and [[198,18,10]], which are competitive with state-of-the-art constructions. These codes admit a directly addressable logical basis, enabling highly parallel logical measurement layers, and feature simple logical operators. We further present properties of a family of planar qLDPC codes that achieve parameters as attractive as permitted by known no-go theorems

[6]. We will also address the challenging problem of decoding [7,8], which corresponds to the classical task of determining suitable corrections from syndrome information. Finally, an outlook will highlight future directions for the field, including just-in-time decoding for high-threshold decoding of non-Pauli codes enabling two-dimensional universality [9], as well as a broader discussion of the challenges that lie ahead [10].

[1] Nature Phys. 20, 1648 (2024).
[2] PRX Quantum 6, 010360 (2025).
[3] PRX Quantum 5, 010342 (2024).
[4] Quantum 9, 1905 (2025).
[5] arXiv:2603.05398 (2026).
[6] In preparation (2026).
[7] Nature Comm. 16, 8214 (2025).
[8] PRX Quantum 5, 020349 (2024).
[9] arXiv:2604.02033 (2026).
[10] arXiv:2510.19928 (2025).

Jens Eisert is a theoretical physicist at the Freie Universität Berlin, working on notions of quantum computing and the study of complex quantum systems. He is known for his rigorous work in quantum information science, which spans the traditional fields of physics, mathematics, and computer science, and is pragmatically motivated by application, protocol, or phenomenon. In the past, he has made several important contributions to the field of quantum computing, focusing on what quantum computers can do and their ultimate limitations, making him one of the most seen and cited researchers in his field. Before joining the Freie Universität Berlin, he was a full professor at the University of Potsdam and an assistant professor at Imperial College London. For his work, he has received an ERC AdG, an ERC CoG, a EURYI Award (the predecessor of the ERC StG), and a Google NISQ Award.

Contact: jenseisert@gmail.com

Fast logic for the surface code: a challenge for decoding | Prof. Dr. Barbara M. Terhal, Delft University of Technology / QuTech

Transversal logical gates offer the opportunity for fast and low-noise logic, particularly when interspersed by a single round of parity check measurements of the underlying code. Using such circuits for the surface code requires decoding across logical gates, complicating the decoding task. We show how one can decode across an arbitrary sequence of transversal gates for the unrotated surface code, using a fast "logical observable" minimum-weight perfect matching-based decoder, and benchmark its performance in Clifford circuits under circuit-level noise. We discuss challenges and ideas in generalizing this to windowed logical observable matching decoders.

Barbara Terhal is a professor working at Delft University of Technology and affiliated with QuTech, and the company Riverlane as research fellow. Her research interests are in quantum error correction and in understanding the computational and conceptual novelty of quantum information.

Contact: B.M.Terhal@tudelft.nl

Significantly more efficient Clifford+T synthesis for small-angle rotations and application to Trotterization | Dr. Nick Blunt, Riverlane

It is well known that arbitrary-angle rotations can be implemented fault-tolerantly to arbitrary precision by compilation to a Clifford+T gate set. This approach is scalable, but is generally understood to have a high overhead of tens of T gates per rotation. In this talk, we will describe our work to reduce the cost of Clifford+T synthesis, and its application to significantly reduce the cost of fault-tolerant Trotterization for chemistry problems. Our main tool to investigate this task is taking probability and quasi-probability mixtures of Clifford+T channels. In particular, we show that the T cost to implement a rotation channel can be reduced significantly for small-angle rotations, and returning to existing angle-independent results in the worst case. This dispels the commonly-stated claim that Clifford+T synthesis has a high overhead independent of the rotation angle, and is particularly impactful for Trotter circuits, which are dominated by small-angle rotations.

Using our results, we show that the T-gate cost of Trotter circuits compiled to Clifford+T gates becomes constant in the limit of small Trotter step sizes, and can be reduced by orders of magnitude even for large step sizes. Our results are also important for early fault-tolerant quantum computers, as they allow rotations to be implemented with shorter Clifford+T sequences, and should allow more straightforward incorporation of error mitigation.

Nick Blunt is a Staff Quantum Scientist at Riverlane, where he has been since 2021. His current research focusses on early fault-tolerant quantum computing, including quantum algorithms, applications and compilation for early error-corrected devices. Previously, he completed his PhD at the University of Cambridge, held a Research Fellowship at St John's College, Cambridge, and completed a postdoc at UC Berkeley, where he worked on developing quantum Monte Carlo methods and electronic structure theory.

Contact: nick.blunt@riverlane.com

End-to-End Efficiency in Dissipative Preparation of Thermal and Ground States | Prof. Lin Lin, University of California, Berkeley / Caltech

Inspired by natural cooling processes, dissipation has emerged as a powerful paradigm for preparing low-energy states of quantum systems, including thermal and ground states. In contrast to traditional quantum algorithms that rely on coherent evolution followed by final measurement and postselection, dissipative state preparation involves repeated mid-circuit measurements. This makes runtime analysis significantly more challenging, especially for non-commuting Hamiltonians. Recent advances, such as the development of Kubo-Martin-Schwinger (KMS) detailed-balanced Lindbladians and protocols for dissipative ground state preparation, have enabled not only efficient algorithms, as measured by the simulation cost per unit time, but also end-to-end runtime guarantees, as measured by the mixing time—the timescale required to reach the target quantum state from any initial state. In certain cases, sharp estimates on mixing times can be rigorously established. I will present these developments, and discuss how to simplify such protocols for efficient implementation on early fault-tolerant quantum devices while maintaining end-to-end efficiency.

Lin Lin is a Professor of Mathematics at UC Berkeley and a Senior Faculty Scientist at Lawrence Berkeley National Laboratory. He has received the Sloan Research Fellowship, NSF CAREER Award, DOE Early Career Award, SIAM CSE Early Career Award, Presidential Early Career Awards for Scientists and Engineers, ACM Gordon Bell Prize (Team), and Simons Investigator award. He is a SIAM Fellow (2026) and an invited speaker at the 2026 International Congress of Mathematicians.

Contact: linlin@math.berkeley.edu

Utility-scale electronic structure with under 100k physical qubits | Dr. Guang Hao Low, Google Quantum AI

We present a quantum code implementable on a regular 2D grid with nearest-neighbor interactions with an estimated encoding rate up to $4.5\times$ of a rotated surface code patch using circuit-level noise in a one- and two-qubit 10^{-3} error uniform depolarizing model. Assuming a 1μs surface code cycle time and a 10μs reaction time, and together with highly-optimized quantum circuits compiled to fault-tolerant QEC primitives, these developments enable chemically accurate ground state phase estimation of a broad class of `utility-scale' electronic structure simulation problems such as the 108 spin-orbital FeMoco-based Nitrogen-fixation catalyst in under a week using fewer than 100k noisy superconducting qubits. We elucidate a pareto frontier of space-time trade-offs and find a minimum physical quantum volume of ≈1 mega-qubit-hour. These correspond to a $>30\times$ space and $>5\times$ spacetime improvement respectively over our previous state-of-art (Physical Review X 15 (4), 041016) minimum-Toffoli resource estimates.

Guang Hao Low is a Staff Research Scientist at Google Quantum AI researching topics related to the scalable and practical quantum simulation of many-body systems, with expertise spanning applications, algorithms, and compilation. Before joining Google in 2024, Guang Hao was a Principal Researcher at Microsoft Azure Quantum focusing on applications of quantum computers to chemistry, and before in 2017 graduated from the Massachusetts Institute of Technology in Professor Isaac L. Chuang's research group with a PhD in Physics with notable work including Quantum Signal Processing and Qubitization.

Contact: guanghaolow@gmail.com

Robust characterization of average gate set noise and cross-talk using gate-set shadows | Jadwiga Wilkens, Johannes Kepler University Linz

As quantum processors scale, robust and scalable tools to characterize gate-level noise become indispensable. Randomized benchmarking (RB) and its many variants have emerged as the go-to protocols in practice: it yields a single number to characterize a gate set, the average gate fidelity, per irreducible subspace. It has been argued that RB can in principle be extended into a full tomographic framework (RB tomography), but large scale practical implementations even of partial tomographic information have long been hindered by the need for sequence inversion, explicit gate interleaving, and an the required measurement statistics. In this talk, we report on scalable implementations of a flexible and efficient variant of RB tomography called gate-set shadows on super-conducting qubit computing platforms. From one efficiently implemented randomized circuit experiment, we reconstruct marginals of the average noise channel, learn classically correlated quantum noise, including cross-talk, and infer a variety of diagnostic information and performance metrics.

Jadwiga Wilkens studied Physics at Freie Universität Berlin, completing both her Bachelor's and Master's degrees under the supervision of Jens Eisert. After a research internship at TII in Abu Dhabi,, where she worked on characterizing superconducting qubits and the open-source quantum computing software Qibo, she joined Richard Küng's group at Johannes Kepler University Linz as a PhD student in 2023. Her research develops practical methods for benchmarking, characterizing, and mitigating errors in quantum devices. She works on classical shadow tomography, including gate-set shadows and robust shadow protocols, and currently develops scalable techniques for crosstalk tomography and data-driven analysis of large experimental datasets from quantum hardware.

Contact: jadwiga.wilkens@jku.at

Learning to predict ground state properties of gapped Hamiltonians | Prof. Dr. Richard Kueng, Johannes Kepler University Linz

Classical machine learning (ML) provides a potentially powerful approach to solving challenging quantum many-body problems in physics, chemistry and material science. However, the advantages of ML over traditional methods have not been firmly established. In a series of works, we prove that classical ML algorithms can efficiently predict ground-state properties of gapped Hamiltonians after learning from other Hamiltonians in the same quantum phase of matter. By contrast, under a widely accepted conjecture, classical algorithms that do not learn from data cannot achieve the same guarantee.

Our proof technique combines mathematical signal processing with quantum many-body physics and also builds upon the recently developed framework of classical shadows. I will try to convey the main proof ingredients and also present numerical experiments that address the anti-ferromagnetic Heisenberg model and Rydberg atom systems.
This is joint work with Hsin-Yuan (Robert) Huang, Giacomo Torlai, Victor Albert, Laura Lewis, Viet Tran and John Preskill.

Richard Kueng is currently the head of the department for quantum computing at the Johannes Kepler University Linz and an elected member of the Young Austrian Academy of Sciences. Beforere turning to his hometown Linz in 2020, he spent almost 15 years studying andworking abroad: Zuerich, Cambridge, Freiburg, Sydney, Cologne, Berlin, Los Angeles. From 2017-2020 he was a researcher at the California Institute of Technology, where he collaborated closely with Google and Amazon. There he also co-developed the classical shadow formalism—a new quantum-classical interface that made a lasting impact on modern quantum technologies.

Contact: richard.kueng@jku.at

Towards fault tolerant quantum computation on the Rydberg platform | Prof. Dr. Hans Peter Büchler, University of Stuttgart

A quantum computer based on Rydberg atoms exhibit a few features, which are unique to this platform. In this talk, I will introduce the platform of Rydberg quantum computer and will review the latest progress and achievements on this platform. Especially, this will include the discussion on quantum many-body gates as well as the shuttling operation of atoms, which allows for changing the connectivity of the qubits during run time of a quantum algorithm. A special focus will be on the latest results and approaches towards fault tolerant quantum computation on this platform.

Prof. Dr. sc. nat. Hans Peter Büchler is Professor of Physics and head of the Institute for Theoretical Physics III at the University of Stuttgart. He received his PhD at the ETH in Zürich in the group of Prof. G. Blatter in 2003 and after a postdoc stay at the University of Innsbruck in the group of Prof. Zoller, he was appointed as professor at the University of Stuttgart in 2007. His research focus in on quantum many-body systems realized with artifical matter such as cold atomic gases, polar molecules, and Rydberg atoms. A special focus is on research on quantum computation with Rydberg atoms.

Contact: buechler@theo3.physik.uni-stuttgart.de

Path to Starling – Realizing fault-tolerant quantum computation at scale | Dr. Tristan Müller, IBM Research Ehningen

Realizing large-scale, fault-tolerant quantum computing is essential for executing advanced quantum algorithms whose gate requirements exceed the capabilities of today's devices by several orders of magnitude. In this talk, I will present IBM's roadmap toward Starling, a fault-tolerant quantum computer targeted for 2029 and designed to support 200 logical qubits. I will highlight key recent milestones, including the development of bivariate bicycle codes and the bicycle architecture, which together significantly reduce the qubit overhead traditionally required for fault tolerance. I will also share our latest progress on real-time decoding of bivariate bicycle codes using Relay-BP. The talk concludes with an outlook on current and future technical challenges on our path to Starling.

Tristan Müller joined IBM in April 2020 and is currently leading a team focusing on real-time decoding algorithms for quantum error correction at IBM R&D in Ehningen. Before joining IBM, Tristan studied Physics at RWTH Aachen, where he wrote his Master's thesis on superconducting magnetic sensors. Afterwards, he was a graduate student at the Max Planck Institute of Microstructure Physics, where he completed his PhD thesis on the simulation of ultrafast and ultra long-ranged quantum systems.

Contact: tristan.mueller@ibm.com

Leveraging low energy assumptions for quantum speedups | Dr. Nicholas Rubin, Google Quantum AI

We present a method of integrating low-energy assumptions into a variety of quantum algorithms for physical simulation that leverages Hamiltonians represented as a sum of squares and spectral amplification. Spectral amplification minimizes query costs by useful uncertainty propagation when performing a parameter estimation task if the initial state is in the low-energy sector of a non-negative Hamiltonian. The non-negative Hamiltonian representations we utilize are sum-of-squares certificates on the lowest eigenvalue. This work connects non-commutative polynomial optimization to quantum algorithms and is demonstrated to lower quantum gate complexities when computing the ground state of strongly correlated electronic systems in first and second quantization. We will also highlight how sum-of-squares Hamiltonian representations can be used in classical electronic structure simulation with potentially reduced costs.

Nicholas Rubin is a Staff Scientist at Google Quantum AI. His work primarily focuses on physical simulation algorithms for fault-tolerant quantum computers. Prior to Google, Nicholas was a research scientist at Rigetti computing and worked on efficient fermionic tomography. Nicholas holds a PhD in Chemistry from the University of Chicago and a Bachelors of Science from the University of Illinois at Urbana-Champaign.

Contact: nickrubin@google.com

Fitting quantum chemistry simulations of early fault tolerant quantum computers | Dr. Christian Gogolin, Covestro

It is intuitively plausible and widely believed that quantum computers are naturally good at simulating other quantum many-body systems such as those relevant in statistical mechanics, condensed matter physics, and chemistry. But is that actually true? How far are we from running such simulations on early fault-tolerant machines? How confidently and on what level of abstraction can we estimate the quantum resources required, and will quantum break even with classical in runtime and system size regime that is practically relevant. In this talk I will try (at least partially) answer some of these questions and present so of the relevant recent results from the quantum computing group at Covestro.

Christian Gogolin works at the intersection of quantum information science, quantum computing, and many-body physics. With extensive experience in software development, computational chemistry, high-performance computing, and quantum algorithms, Christian has contributed to over 45 scientific publications. As Head of High Performance & Quantum Computing in Covestro's Digital R&D department and Founder and Executive Board member of „Quantum - the open journal for quantum science", he has led distributed teams and helped shape innovative approaches to scientific computing and publishing. Christian brings expertise spanning research, programming, leadership, and digital infrastructure development, alongside a strong interest in user-centered design and impact-oriented science.

Contact: christian.gogolin@covestro.com

From Quantum Algorithms to Better Therapies and Materials: Transitioning from Near-Term to Early Fault-Tolerant Impact in Life Sciences and Materials Discovery | Dr. Stefan Knecht, Algorithmiq

Quantum computing is at the threshold of transforming molecular simulation, offering solutions to some of the most intractable challenges in computational chemistry. One of the areas where this transformation is urgently needed is photodynamic therapy (PDT) drug discovery, a highly promising approach to targeted cancer treatment. PDT drugs must be carefully designed to optimize light absorption, reactive oxygen species generation, and excited-state stability. In this talk, I will outline our project, awarded as the sole winner of the Wellcome Leap Quantum4Bio Global Challenge [1] that is designed to address these challenges by building the first scalable quantum simulation pipeline for PDT drug discovery, allowing for the rational design of next-generation photosensitizers. In particular, I will discuss a series of groundbreaking advancements, enabling largescale quantum chemistry simulations that were previously infeasible and setting the stage for the first credible demonstration of useful quantum advantage in molecular modelling.
With these innovations at hand, I will present an end-to-end procedure —from defining a molecular structure to computing error-mitigated and error-corrected ground- and excited-state energies as well as molecular properties for molecules and materials using contemporary quantum hardware at a 50+ qubit scale. This marks a significant step towards practical, early-fault tolerant hardware-compatible quantum chemistry simulations for molecular systems as well as materials.

[1] https://wellcomeleap.org/q4bio_prize_announcement/

Dr. Stefan Knecht is the Head of Quantum & R&D Integration and Execution at Algorithmiq, where he leads efforts to bridge cutting-edge theoretical research with real-world applications, contributing to the advancement of quantum-enabled solutions in science and industry. His work centers on leveraging quantum computing to solve complex molecular and simulation challenges, particularly in areas such as drug discovery and photodynamic therapy. He holds a PhD in Theoretical Chemistry and completed his habilitation at ETH Zürich. Throughout his career, he has worked at several leading European research institutions, building expertise in high-performance computing and advanced quantum chemistry methods.

Contact: stefan@algorithmiq.fi

Pauli and Majorana Propagation Methods for Supporting Chemistry and Materials Workflows on Quantum Hardware | Prof. Zoë Holmes, EPFL

Simulating quantum circuits classically is in general a hard task. However, certain families of quantum circuits may be practically or even provably efficiently simulable by use of specialized classical algorithms. Following on from Stefan Knecht's talk on Algorithmiq's end-to-end pipeline for quantum chemistry, this talk will focus on the role that such classical simulation methods can play within this pipeline, in particular for designing state-preparation circuits. We will cover Pauli propagation, which has recently been shown to enable efficient classical simulation of expectation values in quantum circuits and a wide range of noise-free quantum circuits. We will then discuss a generalization of this approach to fermionic systems via Majorana propagation, opening up new applications in quantum chemistry and materials science. In particular, we will discuss how propagation-based methods can be used to help construct approximate ground-state circuits, and how they can be efficiently combined with other classical and quantum subroutines in order to point towards promising applications of quantum devices.

Zoë Holmes is a tenure-track Assistant Professor of Physics at EPFL, where she founded the Laboratory of Quantum Information and Computation in 2022. Alongside her EPFL role, she works part-time as a Senior Researcher at Algorithmiq. Her research focuses on quantum and classical algorithms for quantum computing. Before joining EPFL, she was a postdoctoral researcher and Mark Kac Fellow at Los Alamos National Laboratory. She completed her PhD in quantum thermodynamics at Imperial College London in 2020, after obtaining a master's degree in Physics and Philosophy from the University of Oxford.

Contact: zoe.holmes@epfl.ch

Parallel Quantum Chemistry on NISQ Computers: From RDMFT Subsystems to Embedded Materials | Prof. Thomas Kühne, CASUS

„A central obstacle for quantum chemistry on near-term quantum computers is not only the noise of present devices, but the size of chemically meaningful electronic-structure problems. We proposed a parallel hybrid quantum-classical algorithm based on reduced density-matrix functional theory (RDMFT) and the adaptive cluster approximation. Instead of mapping the full many-electron problem onto one large quantum circuit, the density-matrix functional is decomposed into a set of indirectly coupled subsystem functionals. Each subsystem can then be solved by a variational quantum algorithm, while the independence of the subsystem problems opens a natural route to parallel execution and reduces the qubit requirements per quantum processor.
In this talk I will present the main ideas behind this approach, its relation to variational quantum eigensolvers, and its demonstration for Hubbard-like systems on IBM superconducting quantum hardware. I will discuss how the method trades one monolithic quantum chemistry calculation for many smaller constrained minimization problems, and why this matters for NISQ-era devices with limited qubit counts, circuit depths, and coherence times.
I will then connect this perspective to our current work on CP2K active-space embedding for periodic battery materials. There, the same guiding principle reappears in a chemically more realistic form: isolate the strongly correlated local degrees of freedom, keep the environment classical, and use exact or quantum solvers only where they are needed. This provides a bridge from the original RDMFT-based parallel quantum chemistry concept toward practical quantum-computing-inspired workflows for materials simulations.“

Prof. Dr. Sc. ETH Thomas D. Kühne is Founding Director of the Center for Advanced Systems Understanding (CASUS) at Helmholtz-Zentrum Dresden-Rossendorf (HZDR) and Professor of Computational Systems Science at TU Dresden. He studied Computer Science and Computational Science and Engineering at ETH Zürich and earned his doctoral degree in Theoretical Physics under the supervision of Michele Parrinello. Following postdoctoral research at Harvard University, he held faculty positions at the University of Mainz and Paderborn University, where he became Full Professor of Theoretical Chemistry.
His research focuses on the development of advanced methods for ab initio molecular dynamics and electronic structure theory, as well as their application to complex condensed-phase systems in chemistry, biophysics, and materials science. He is a core developer of the CP2K and i-PI simulation packages. His work spans aqueous interfaces, confined water, catalysis, energy materials, and sustainable technologies. He has authored more than 200 peer-reviewed publications and received an ERC Starting Grant for research on "on-water" catalysis.

Contact: t.kuehne@hzdr.de

A framework for spin-adapted quantum chemistry on quantum computers | Dr. Nathan Fitzpatrick, Quantinuum

Quantum computers promise to transform molecular simulation, but many existing algorithms overlook the powerful role of spin symmetry in chemistry. The Quantum Paldus Transform provides a new framework that makes spin adaptation a built-in feature of quantum computation.
At its core, the transform connects two representations of electronic states: the conventional occupation-number basis used in quantum chemistry, and a symmetry-adapted basis that organises states by total spin, particle number, and orbital symmetries. This shift, grounded in mathematical structure known as Paldus duality, allows quantum devices to work directly with spin-pure states - the natural language of chemistry.
The benefits are considerable. Spin-free Hamiltonians reduce to block-diagonal, sparser forms, enabling more efficient simulations. The transform itself admits polynomial-cost implementations and even highly compact circuit constructions. Beyond simulation, the framework facilitates efficient preparation of Configuration State Functions (CSFs) and naturally embeds quantum information in decoherence-free subsystems, offering potential protection against certain noise channels.
By extending the quantum Schur transform into the fermionic setting, the Quantum Paldus Transform establishes a principled and practical route for exploiting spin symmetry in quantum algorithms. This framework opens new directions for scalable, accurate, and symmetry-aware quantum chemistry algorithms on quantum computers.

Nathan Fitzpatrick is a Lead Research Manager at Quantinuum, where he has worked for the past seven years (formerly Cambridge Quantum Computing). He leads a research group focused on leveraging symmetries to enhance quantum simulation and algorithms, with particular applications in quantum chemistry. His interests include compiling these algorithms down to the circuit level, and he heads the development of algorithmic extensions for the guppy software package. Nathan earned his PhD at Imperial College London under the supervision of Prof. Mike Robb FRS and Prof. Mike Bearpark, where his research explored the theoretical foundations of configuration interaction under global SU(2) symmetry.

Contact: nathan.fitzpatrick@quantinuum.com

One and Many-Body Aspects of Electronic Structure on Quantum Computers | Prof. Dr. Jakob Kottmann, University of Augsburg

Quantum computation is currently at a stage where the applicability of quantum algorithms appears imminent, but their full potential remains an open question. A significant fraction of present-day quantum algorithmic research relies on numerical procedures to gain further insights and explore new applications. Here, one typically deals with numerous interconnected classical and quantum algorithmic components. In this talk, I will illustrate how quantum algorithmics and scientific software development can form a powerful symbiosis to tackle problems in electronic structure and other potential applications of quantum computers.

Jakob S. Kottmann is a professor of quantum algorithmics at the Computer Science Institute, University of Augsburg (Germany).
His research lies in the intersection of quantum algorithmics, quantum chemistry and scientific software development.

Contact: jakob.kottmann@uni-a.de

Spectroscopy use cases for fault-tolerant quantum computing | Dr. Jan Reiner, HQS Quantum Simulations

Finding and realizing productive use cases is a pressing problem for the field of quantum computation. Identifying problems that are both relevant and genuinely better suited to quantum computation than classical alternatives remains a central challenge. Without more compelling, concrete applications, the promise of fault-tolerant quantum computing risks remaining mostly theoretical. I will argue for use cases within the realm of spectroscopy. At its core, spectroscopy probes the response of a quantum mechanical system to external perturbations — a process governed by real-time dynamics. Computing spectral functions therefore requires simulating the time evolution of quantum states, a task that is natural for a quantum computer, yet difficult for classical methods in general. I will show explicit examples of industrially relevant spectroscopy use cases and estimate the applicability of fault-tolerant quantum computing to perform their underlying calculations.

Jan Reiner obtained his Ph.D. at KIT's Institute of Theoretical Solid State Physics in the group of Gerd Schön on the topic of quantum simulation, computation and information. Towards the end of his studies he co-founded HQS Quantum Simulations, where he now holds the title of Chief Scientific Officer. As CSO, his central responsibility is the oversight of HQS' scientific work specifically in the context of the quantum computing efforts of the company.

Contact: jan.reiner@quantumsimulations.de

Near-term and fault-tolerant quantum computing applications in the natural sciences | Dr. Ivano Tavernelli, IBM Quantum

Quantum computing is entering a new phase, moving from noisy intermediate-scale devices toward fault-tolerant architectures capable of delivering scalable and reliable quantum advantage. Within this evolving landscape, significant progress has been made in the design of algorithms and workflows that bridge near-term capabilities with long-term fault-tolerant quantum computing. In particular, the development of resource-efficient quantum algorithms, together with error-mitigation and early error-correction techniques, is paving the way toward practical applications aligned with the fault-tolerant roadmap pursued by IBM. In this talk, I will also briefly outline IBM's roadmap toward fault-tolerant quantum architectures and the corresponding implications for algorithm design. From an application perspective, near-term and fault-tolerant quantum computing is expected to unlock transformative capabilities across a wide range of domains. These include combinatorial optimization and machine learning, as well as applications in healthcare and life sciences such as molecular modeling and drug discovery. In the physical sciences, quantum algorithms targeting quantum chemistry, materials science, and lattice gauge theories in high-energy physics are particularly promising, as will be outlined in this talk. Many of these problems remain fundamentally beyond the reach of classical methods due to the exponential complexity of strongly correlated and high-dimensional systems. Near-term and fault-tolerant quantum algorithms, enabled by robust logical qubits and scalable architectures, offer a pathway to address these challenges, with the potential to provide accurate simulations of complex molecular processes, many-body quantum systems, and fundamental physical phenomena.

Ivano Tavernelli is a Senior Research Staff Member in Quantum Computing at IBM Research – Zurich. Since 2018, he has served as IBM's Global Leader for Advanced Algorithms in Quantum Simulations, where he is responsible for driving research and applications in physics, chemistry, biology, and materials science. His work focuses on the design of efficient and scalable quantum algorithms for both near-term and fault-tolerant quantum computing. Prior to joining IBM, he held a postdoctoral fellowship at the University of Cambridge (UK) and subsequently served as Maître d'Enseignement et de Recherche at the École Polytechnique Fédérale de Lausanne (EPFL). He holds two Master's degrees, in Biochemistry and Theoretical Physics, from ETH Zurich, as well as a PhD in Natural Sciences from ETH Zurich.

Contact: ita@zurich.ibm.com

Imaginary-time evolution in the age of quantum computing | Dr. Fedor Šimkovic, IQM Quantum Computers

Imaginary-time evolution (ITE) is a central framework for computing ground states of quantum systems, with broad applications in condensed matter physics, quantum chemistry, and related fields. Many variants of ITE have been developed, including approaches based on tensor networks and quantum Monte Carlo. On quantum computers, however, a direct implementation of ITE is obstructed by its intrinsically non-unitary character. This challenge has motivated a rapidly growing body of quantum and hybrid quantum-classical algorithms designed to emulate or approximate imaginary-time dynamics.
In this talk, Šimkovic will review recent progress in ITE methods for quantum computers and present several of their contributions to this area. He will first discuss an operator-projected formulation of variational quantum imaginary-time evolution, combined with Majorana propagation. He will then describe hybrid stochastic algorithms inspired by auxiliary-field quantum Monte Carlo and full configuration-interaction quantum Monte Carlo. Next, he will introduce a stochastic implementation of ITE based on quantum signal processing primitives. Finally, he will give a short introduction to the augmented ITE formalism, which can dramatically accelerate convergence relative to standard ITE and may have implications across a broad range of imaginary-time evolution methods.

Fedor Šimkovic received his Diplom in Physics from the University of Tübingen and his PhD from King's College London, where he worked on diagrammatic Monte Carlo methods for condensed matter systems. He then held a joint postdoctoral position between École Polytechnique and Collège de France in Paris, focusing on quantum Monte Carlo and embedding methods. He subsequently spent four years at the quantum computing startup IQM, in senior research and leadership roles, most recently as Head of Algorithms and Applications. His current interests center on developing quantum algorithms for problems in physics and chemistry.

Contact: fedor.simkovic@meetiqm.com

Scientific Challenges to Apply Quantum Computing in Drug Design | Dr. Michael Streif, Boehringer Ingelheim

Quantum computers hold the promise of outperforming classical systems and are widely regarded as the future of quantum chemistry and drug design. However, realizing this potential in real-world pharmaceutical applications requires addressing a far broader set of challenges than those typically explored - well beyond ground-state energy calculations for single molecules. In this talk, we examine the scientific challenges that must be overcome to make quantum computing a practical tool for drug design. We will share our latest work on fault-tolerant algorithms and discuss strategies for tackling these challenges.

Michael Streif is a Quantum Computing Scientist at Boehringer Ingelheim, working on how quantum computing could help accelerate the process of drug discovery.
Prior to joining Boehringer Ingelheim, Michael studied in Freiburg and Oxford and later earned his Ph.D. in physics at FAU Erlangen-Nuremberg, where he developed quantum algorithms for complex optimization problems. He worked on developing quantum algorithms at Volkswagen and NASA Ames Research Center, contributing to advancements in quantum computing for real-world applications.

Contact: michael.streif@boehringer-ingelheim.com

Contributed Talks

Polylogarithmic-Depth Quantum Algorithm for Simulating the Extended Hubbard Model on a Two-Dimensional Lattice Using the Fast Multipole Method | Yu Wang, Technical University of Munich

The extended Hubbard model on a two-dimensional lattice captures key physical phenomena, but is challenging to simulate due to the presence of long-range interactions. In this work, we present an efficient quantum algorithm for simulating the time evolution of this model. Our approach, inspired by the fast multipole method, approximates pairwise interactions by interactions between hierarchical levels of coarse-graining boxes. We discuss how to leverage recent advances in two-dimensional neutral atom quantum computing, supporting non-local operations such as long-range gates and shuttling. The resulting circuit depth for a single Trotter step scales polylogarithmically with system size.

Yu Wang is a PhD candidate in physics at the Technical University of Munich (TUM), supervised by Prof. Dr. Christian B. Mendl. His research focuses on quantum algorithms and tensor network methods, with particular interest in the simulation of strongly correlated quantum systems. He received both his bachelor's and master's degrees in physics from Lanzhou University and TUM, respectively.

Contact: 18yu.wang@tum.de

Addressable fault-tolerant universal quantum gate operations for high-rate lift-connected surface codes | Dr. Sascha Heußen, neQxt

Quantum low-density parity check (qLDPC) codes are among the leading candidates to realize error-corrected quantum memories with low qubit overhead. Potentially high encoding rates and large distance relative to their block size make them appealing for practical suppression of noise in near-term quantum computers. In addition to increased qubit-connectivity requirements compared to more conventional topological quantum error correcting codes, qLDPC codes remain notoriously hard to compute with. In this work, we introduce a construction to implement all Clifford quantum gate operations on the recently introduced lift-connected surface (LCS) codes (Old et al. 2024). These codes can be implemented in a 3D-local architecture and achieve asymptotic scaling [[n, \mathcal{O}(n^{1/3}), \mathcal{O}(n^{1/3})]]. In particular, LCS codes realize favorable instances with small numbers of qubits: For the [[15,3,3]] LCS code, we provide deterministic fault-tolerant (FT) circuits of the logical gate set \{\overline{H}_i, \overline{H}_i, \overline{C_i X_j}\}_{i,j \in (0,1,2)} based on flag qubits. By adding a procedure for FT magic state preparation, we show quantitatively how to realize an FT universal gate set in d=3 LCS codes. Numerical simulations indicate that our gate constructions can attain pseudothresholds in the range p_{\mathrm{th}} \approx 4.8\cdot 10^{-3}-1.2\cdot 10^{-2} for circuit-level noise. The schemes use a moderate number of qubits and are therefore feasible for near-term experiments, facilitating progress for fault-tolerant error corrected logic in high-rate qLPDC codes.

Sascha Heußen is a postdoc-level research scientist. His interests are in small-scale fault tolerance and near-term implementations of quantum error correction. This matters because ultra-high-fidelity qubits are needed to practically implement quantum algorithms that are actually useful and cannot be simulated on classical computers. His current affiliation is with neQxt [nɛkst], an ion-trap quantum computing company. I am based in Cologne, Germany. Heußen's dissertation from RWTH Aachen was awarded the Quantum Future Award in 2024 by the German Federal Ministry of Education and Research. I am leading the project snaQCs2025, funded by the German Federal Ministry of Research, Technology and Space.

Contact: s.heussen@neqxt.org

Logarithmic-depth quantum state preparation of polynomials | Dr. César Feniou, Qubit Pharmaceuticals

Quantum state preparation is a central primitive in many quantum algorithms, yet it is generally resource intensive, with efficient constructions known only for structured families of states. This work introduces a method for preparing quantum states whose amplitudes are given by a degree-d polynomial, using circuits with logarithmic depth in the number n of qubits and only O(n) ancilla qubits, improving previous approaches that required linear-depth circuits. The construction first relies on a block-encoding of an affine diagonal operator based on its Pauli-basis decomposition, which involves only n terms. A modified linear-combination-of-unitaries (LCU) technique is introduced to implement this decomposition in logarithmic depth, together with a novel circuit for the EXACT-one oracle that flags basis states in which exactly one qubit is in the state |1> . It then uses a generalized quantum eigenvalue transformation (GQET) to promote this affine operator to an arbitrary degree polynomial. Theoretical analysis and numerical simulations are reported along with a proof-of-principle implementation on a trapped-ion quantum processor using 14 qubits and more than 500 primitive quantum gates. Because polynomial approximations are ubiquitous in scientific computing, this construction provides a scalable and resource-efficient approach to quantum state preparation, further improving the potential of quantum algorithms in fields such as chemistry, physics, engineering, and finance.

César Feniou obtained his PhD in chemistry from Sorbonne Université and is currently a Lead Quantum Algorithm Scientist at Qubit Pharmaceuticals. His research focuses on quantum algorithms for many-body systems, with an emphasis on bridging efficient quantum routines with realistic electronic structure problems toward practical quantum advantage.

Contact: cesar.feniou@gmail.com

Fast simulations of the Fermi-Hubbard model on the SPOQC architecture | Théo Dessertaine, Quandela

Fault tolerance is essential for large-scale, reliable quantum computation, yet the substantial resource overhead associated with quantum error correction (QEC), including encoding, syndrome extraction, decoding, and fault-tolerant gate synthesis, remains a major challenge. Logical-level resource estimation is therefore crucial for realistic assessments of quantum advantage.

In this work, we analyze the resource requirements of the SPOQC architecture, a hybrid spin–photon platform with several features advantageous for fault-tolerant quantum computing. First, it enables direct parity measurements, allowing ancilla-free implementations of dynamical QEC codes such as the Honeycomb Floquet code, currently the best-performing code for this platform. Second, photon-mediated two-qubit operations extend connectivity beyond a 2D nearest-neighbor layout, enabling more resource-efficient QEC schemes. Third, fast QEC cycles reduce runtime, an important advantage for deep fault-tolerant circuits.

Exploiting these features, we propose a bi-planar honeycomb qubit layout. Each plane hosts Honeycomb Floquet patches requiring only three nearest-neighbor connections per qubit, with logical gates implemented via lattice surgery. Qubits across planes are pairwise connected, enabling transversal CNOT and SWAP gates. This structure can operate as memory–workspace modules or support optimized, problem-specific compilations.

We apply this layout to the simulation of the $L\times L$ Fermi–Hubbard model using the plaquette-based Trotterization (PLAQ) algorithm with L^2-parallel compilation. Aligning the hardware layout with the Hamiltonian structure eliminates fermionic swaps and exploits transversal inter-plane connections. Each Trotter step requires $4\sigma+90$ logical time steps, compared to $6\sigma+354$ in previous single-plane implementations. While this parallel approach minimizes spacetime volume, it increases qubit demand due to magic state factories and local fermion-to-qubit mappings. Future work should explore more spatially efficient schemes such as Serial PLAQ and L-parallel PLAQ.

Theo Dessertaine is a researcher in Quantum Error Correction and Fault-Tolerance at Quandela, a French photonic quantum computing company based in the Paris region.

Contact: theo.dessertaine@quandela.com

Reformulating Quantum Imaginary-Time Evolution via Curvature and Higher-Order Statistical Information | Dr. Carlos Benavides-Riveros, IQM Quantum Computers

Preparing quantum ground states efficiently is a central challenge in quantum simulation and quantum optimization. Quantum imaginary-time evolution (QITE) offers a powerful, ansatz-free route to this goal, with guaranteed asymptotic convergence; yet in practice it suffers from prohibitively slow convergence and fundamental difficulties in quantum implementation arising from its non-unitary character. Here we introduce a curvature-driven reformulation of QITE that overcomes these limitations by systematically exploiting geometric and higher-order statistical information about the energy landscape. Rather than following the energy-variance alone, our method identifies locally superexponential descent directions, yielding accelerated late-time convergence with substantially fewer evolution steps and final states of improved statistical quality — all without sacrificing the ansatz-free character of the original approach. We demonstrate that this curvature-driven framework enables efficient, scalable ground-state preparation across a range of quantum systems, opening new avenues for practical quantum simulation and optimization.

Carlos Benavides-Riveros Quantum Algorithm Engineer at IQM Quantum Computers. Marie Skłodowska-Curie Fellow (2022–2024). Member of the Royal Society of Chemistry. Formerly at Max Planck Institute for the Physics of Complex Systems (Dresden) and Inspiration-Q (Madrid).
ORCID: https://orcid.org/0000-0001-6924-727

Contact: carlos.benavides@meetiqm.com

Quantum Dynamics: The Next Frontier of Quantum Applications | Danial Motlagh, Xanadu Quantum Technologies

The current landscape of quantum applications presents a fundamental challenge. High-impact proposals, such as large-scale electronic structure calculations, face a long and costly path to realization due to their large resource requirements, while proposals for applications with a shorter horizon, such as simulation of spin models, are not generally believed to result in transformative impact. Quantum dynamics stands out as a domain where the tradeoff between resource requirements and impact becomes far more favorable. Classically, simulating real time quantum dynamics is significantly harder than static problems, widening the gap between classical and quantum methods, and enabling quantum advantage at smaller system sizes. This translates directly to lower resource demands for meaningful applications. At the same time, these simulations remain highly impactful as many key functional properties of materials, such as charge and energy transfer, are inherently dynamical. In this talk I will present our vision for industrial and scientific applications of quantum computers based on simulations of quantum dynamics, and some of our recent technical results in this direction such as our algorithms for simulating vibronic dynamics, non-adiabatic dynamics at metallic surfaces, and chemical dynamics.

Danial Motlagh leads the algorithms and applications R&D efforts at Xanadu. His team focuses on identifying cutting-edge applications of quantum computers and developing algorithms to efficiently executing them on future hardware.

Contact: danial.motlagh@xanadu.ai

Bypassing the Condition Number: Near-Optimal Quantum Solvers for Stationary PDEs | Matthias Deiml, University of Augsburg

We develop a quantum solver for the Poisson equation, a fundamental building block in scientific simulation and a central benchmark for large-scale computational methods. Our algorithm achieves highly favorable scaling: the number of grid points enters the complexity only logarithmically, while the cost of measurement remains linear with respect to the desired accuracy. In the stationary setting, where the absence of time evolution shifts the computational burden to the system's condition number, achieving near-optimal performance requires specialized techniques. We therefore address the input bottleneck for encoding discretized operators and implement a quantum preconditioning scheme specifically designed to control this condition number. We integrate these components into a coherent end-to-end solver, which maps high-level model parameters directly to quantities of interest, providing a concrete and scalable pathway for quantum PDE simulation.

Matthias Deiml is a doctoral researcher at University of Augsburg, specializing in the intersection of quantum information and numerical analysis. His research focuses on developing efficient quantum algorithms for partial differential equations, with a particular interest in nonlinear and stochastic problems.

Contact: matthias.deiml@uni-a.de

Rapid Dissipative Ground State Preparation at Chemical Transition States | Soumya Sarkar, University of Technology Sydney

Simulating chemical reactions is a central challenge in computational chemistry, characterized by an uneven difficulty profile: while equilibrium reactant and product geometries are often classically tractable, intermediate transition states frequently exhibit strong correlation that defies standard approximations. We present a protocol for dissipative ground state preparation that exploits this structure by treating the reaction path itself as a computational primitive. Our protocol uses an approach where a state prepared at a tractable geometry is propagated along a discretized reaction coordinate using Procrustes-aligned orbital rotations and stabilized by engineered dissipative cooling. We show that for reaction paths satisfying a localized Eigenstate Thermalization Hypothesis (ETH) drift condition in the strongly correlated regime, the algorithm prepares ground states of chemical systems with No orbitals to an energy error $ε_E$ with a total gate complexity scaling as $O(N_o^3/ε_E)$. We provide logical resource estimates for benchmark systems including FeMoco, Cytochrome P450, and Ru-based carbon.

Soumya Sarkar is a PhD candidate in quantum computing at the University of Technology Sydney and a Sydney Quantum Academy scholar. His research lies at the intersection of quantum algorithms, computational complexity, and simulation, with a focus on developing efficient quantum methods for studying the physical properties of chemical systems. In particular, he works on problems such as ground-state preparation and time-dynamics simulation. More broadly, he is interested in bridging theoretical advances with practical implementation, especially through rigorous resource estimation and analysis of algorithmic feasibility.

Contact: soumya.sarkar@student.uts.edu.au

Simulating Electron Transfer on Noisy Quantum Computers | Marvin Gajewski, Deutsches Zentrum für Luft- und Raumfahrt (DLR)

We present a framework [1] for the digital-analog simulation of open quantum systems governed by Hamiltonians with linear-vibronic coupling (LVC) and structured vibrational environments. Our approach exploits the intrinsic dissipation of qubits in near-term quantum hardware as a resource to emulate vibrational relaxation, combined with a model-specific error mitigation scheme to filter out noise sources incompatible with the target open system. We validate our strategy by resolving the vibronic transfer spectra of a one-dimensional donor-acceptor chain on IBM superconducting processors, reproducing non-Markovian dynamics and scaling the chain length up to 10 electronic sites, an unprecedented scale for chemical dynamics on quantum computers. Our model of vibronic electron transfer offers a portable, application-oriented benchmark for simulating long-lived entangled states on NISQ computers.

[1] arXiv:2508.18141 (2025), currently in peer review at Nature Communications

Marvin Gajewski studied physics and mathematics at the Technical University Darmstadt. Since 2023, he is a member of the battery research group at DLR Ulm, where he is currently pursuing a PhD focusing on quantum computing and quantum chemistry. His research involves quantum simulations of non-equilibrium dynamics in open quantum systems and microscopic modeling of charge-transfer reactions for electrochemistry.

Contact: marvin.gajewski@dlr.de

Early fault-tolerant resource estimation for ground-state preparation via Lindblad simulation | Dr. Marius Bothe, Riverlane Ltd

Recent advances in algorithms for simulating Lindblad dynamics have clarified their theoretical potential, yet their practicality in early fault tolerant quantum regimes remains uncertain. We address this question by analyzing the single ancilla ground state preparation algorithm of Ding et al. as a representative and broadly useful test case. This method is appealing due to its relevance to common subroutines such as phase estimation and its use of a low overhead dilation construction.

We refine the asymptotic resource analysis of the original work by deriving full prefactors and implementing a Qualtran based costing framework that estimates gate counts for Lindblad evolution to a specified accuracy. To complement these analytic bounds, we perform extensive circuit level simulations of the Hubbard model, an important early fault tolerant application, to obtain empirical error behavior and practical convergence times, which are significantly tighter than worst case theoretical guarantees. We study symmetry preserving mixing operators and further reduce overhead by constructing optimised filter functions that accelerate convergence. Finally, we compile the resulting circuits to fault tolerant architecture.

Together, these results provide a concrete, architecture aware assessment of the feasibility of Lindblad based ground state preparation in the early fault tolerant era, bridging the gap between theoretical constructions and practical implementation.

Marius Bothe finished his PhD at Imperial College London and now works on quantum algorithms development at a joint position between Riverlane and Astex Pharmaceuticals.

Contact: marius.bothe@riverlane.com

Posters

A Local-Wave Basis for the Hubbard Model | Leon Wastl, CASUS / HZDR

The Fermi-Hubbard model is the prototypical model for interacting electrons and can be employed to describe a wide variety of physical phenomena. Its 2D version is believed to contain the fundamental physics describing low-temperature superconductivity. We present a new basis for the two-dimensional Hubbard model which we call the local-wave basis as it is a hybrid between real space and momentum space. We numerically study the advantages of our newly found transformation using the density matrix renormalization group (DMRG). Since DMRG in its more recent form is a method that is inherently one-dimensional as it is built on top of the matrix product state (MPS) formalism, we combine our local-wave basis with a new way of ordering the sites in the MPS based on a modified version of simulated annealing (SA) using the two-site mutual information as its objective function. Combined with this approach to find the optimal ordering, we show that our method yields lower energies for the same maximal bond dimension than both the pure momentum space and the real space formulation in the low to intermediate U/t regime. While we used DMRG for simulations, this new basis might also lend itself well to quantum computing approaches.

Leon Wastl completed his Bachelor's as well as his Masters degree in physics at LMU in Munich. His Masters project in the group of Prof. Schollwöck combined machine learning with both tensor network methods and digital quantum simulation. In June 2025 he joined Dr. Werner Dobrautz's group at CASUS, where he continue to work on novel approaches to numerical methods and quantum simulation to study quantum many-body systems.

Contact: l.wastl@hzdr.de

A Resource-Efficient Reformulation of the Stochastic Projective Quantum Eigensolver | Dr. Prachi Sharma, IQM Quantum Computers

We improved upon the stochastic projective quantum eigensolver [1], a hybrid quantum–classical algorithm that combines stochastic sampling with the projective quantum eigensolver framework to improve convergence and reduce limitations of deterministic approaches.
We propose a reformulation of the estimator that significantly lowers quantum resource requirements by simplifying the measurement process while maintaining accuracy.
We benchmark results on the single Anderson impurity model and hydrogen chains to demonstrate improved efficiency, stable convergence, and good scalability.

1. M.-A. Filip, JCTP, 5964–5981, 2024.

Prachi Sharma Senior Quantum Algorithm Engineer at IQM, focusing on quantum algorithms for chemistry and condensed matter across NISQ and FTQC. Previously a postdoc at the University of Saarbrücken, developing quantum error mitigation methods. Holds a Ph.D. in Physics from the University of Florida and completed a postdoc at the University of Minnesota, researching fermionic dynamical correlations and superconductivity.

Contact: prachi.sharma@iqm.tech

A Transferable Machine Learning Approach to Predict Optimal Orbitals for Electronic Structure Problems |

Abhisshek Yogendra Dubey, Fraunhofer IIS

Variational quantum eigensolvers (VQE) based on the Separable Pair Approximation (SPA) ansatz hold considerable promise for ground-state energy calculations on near-term quantum hardware, yet this calculation strongly depends on the quality of the underlying molecular orbitals. Computing optimized orbital coefficients via classical routines is computationally expensive and must be performed independently for each molecular geometry -- a bottleneck that limits scalability across chemical space. We present a graph neural network (GNN) framework that predicts optimized orbital coefficients directly from molecular geometry and pair-wise bonding structure. Trained on hydrogenic systems of modest size (H_4 and H_6) across tens of thousands of geometries, our model transfer to larger, unseen systems (H_8, H_{10} and H_{12}) without retraining -- demonstrating strong out-of-distribution generalization with respect to system size. On both structured and random geometries, our model can reach mean absolute errors on the order of $\mathcal{O}(1) \ \mathrm{mE_h}$ (milli Hartrees), when evaluated against SPA energies obtained with full classical optimization. Beyond energy estimation, the predicted orbitals serve as high-quality warm-start initializations that substantially reduce optimizer iterations to convergence. Crucially, the optimized orbitals yield shallower SPA ansatz, lowering gate depth and bringing accurate quantum simulations of larger hydrogenic systems within practical reach of current quantum devices. These results establish GNNs as an effective and scalable strategy for accelerating orbital optimization in quantum chemistry workflows.

Abhishek Yogendra Dubey is a Research Associate at Fraunhofer IIS in the Quantum Compilation group, working here for the past 3 years now. His background is in Physics where he also focused on applying Machine Learning techniques to complex problems in Physics. When he is not working on Quantum computing, he is learning the Piano and sometimes reading non-fiction books and Philosophy.

Contact: abhishek.yogendra.dubey@iis.fraunhofer.de

A Unified Benchmarking Study of Variational Quantum Eigensolver Ansatz for Molecular Electronic Structure Problems | Julie Maria Raju, University of Bremen

The Variational Quantum Eigensolver (VQE) has emerged as one of the prominent methods to solve the electronic structure calculations on Noisy-Intermediate scale quantum(NISQ) devices. Despite significant improvement in ansatz design, selecting an optimal ansatz remains a non-trivial task. Existing approaches including chemically inspired ansatz, adaptive schemes and hardware efficient ansätze (HEA) lack a unified comparison. This gap makes the scalability and trade-offs of each method unclear for varying molecular sizes. In this work, we present a comprehensive benchmarking study that evaluates UCCSD, Adapt-VQE and HEA including excitation preserving ansatz under a unified framework. Our analysis focuses on their performance across molecular systems with varying size, evaluating accuracy, circuit depth, and resource requirements under realistic NISQ constraints. This study provides insights into selecting ansatz architectures in VQE, making more resource-efficient quantum simulations on near-term quantum hardware.

Julie Maria Raju is a doctoral researcher at the University of Bremen, Germany. She completed her Master's degree in Physics at FAU Erlangen Nürnberg. Her research interests lie in quantum computing, particularly in variational quantum algorithms, noise analysis, and error mitigation for near term quantum devices. She has worked on hybrid quantum classical models, including quantum convolutional neural networks, during her master thesis at Fraunhofer. Her current work focuses on benchmarking and resource estimation of the Variational Quantum Eigensolver.

Contact: jraju@uni-bremen.de

Benchmarking QCELS for Near-Term Quantum Chemistry Applications | Dr. Fabian Tipp, Fraunhofer IPA / flaQship

Quantum phase estimation algorithms offer a promising route toward obtaining ground state energies in quantum chemistry applications, yet their practical implementation on near-term quantum hardware remains challenging. We present a comprehensive benchmarking study of the Quantum Complex Exponential Least Squares (QCELS) algorithm, systematically investigating its performance characteristics and resource requirements for achieving chemical accuracy.

Using an efficient Qiskit implementation, we conducted exhaustive parameter scans on model Hamiltonians that allow exploration of different correlation regimes, from classical to strongly quantum-mechanical behavior. Key algorithmic parameters were systematically varied, including initial state quality, time evolution parameters, Trotterization depth, and sampling strategies.

Our analysis reveals the interplay between sampling complexity, Trotterization error convergence, and algorithm robustness against imperfect state preparation. We identify optimal parameter regimes that balance computational resources against energy estimation accuracy.

Furthermore, we extend our investigation to include simulated hardware noise models, assessing QCELS performance under realistic error conditions. Preliminary results from small molecular systems executed on actual quantum hardware demonstrate the algorithm's practical applicability and highlight remaining challenges for near-term quantum advantage in chemistry applications.

This work provides practical guidelines for implementing QCELS in quantum chemistry workflows and establishes performance baselines for future algorithmic improvements.

Fabian Tipp studied chemistry at the University of Cologne with a focus on theoretical chemistry, developing a novel multireference coupled cluster method during his master's thesis. He performed his PhD reserach at Forschungszentrum Jülich, where he conducted extensive classical quantum chemistry simulations to identify durable materials for electrochemical energy devices. Currently, he works at Fraunhofer IPA, focusing on the development and benchmarking of quantum algorithms for quantum chemistry applications on near-term quantum hardware.

Contact: fabian.tipp@ipa.fraunhofer.de

Block-encodings as programming abstractions: from gates to polynomials | Matic Petrič, Fraunhofer FOKUS

Quantum computing is nearing practical utility for simulating strongly correlated systems, yet the gate-by-gate design paradigm remains a bottleneck. This seminar explores a shift toward high-level abstractions inspired by the Grand Unification of Quantum Algorithms. We present the foundations of (Generalized) Quantum Signal Processing (GQSP), Singular Value Transformation (GQSVT), and Eigenvalue Transformation (GQET), reframing computation as polynomial transformations of block-encoded matrices.

We demonstrate how Eclipse Qrisp (v0.8) utilizes these techniques via its BlockEncoding class. By allowing for having block encodings as high-level programming abstractions, Qrisp enables researchers to construct block encodings from physical Hamiltonians and manipulate spectra using optimal Chebyshev approximations.

Key Applications for Physics Research:

- Eigenstate Filtering: Applying Gaussian spectral filters via GQSP to isolate ground states in frustrated magnetism, bypassing deep time-evolution circuits.
- Hamiltonian Simulation: Evolving complex many-body systems (e.g., the 1D Heisenberg model) for non-equilibrium dynamics.
- Quantum Linear Systems: We showcase the (near-)optimal linear solver for Dalzell, implemented via GQSVT to solve $Ax=b$ with exponential speedups. This allows for inverting ill-conditioned discrete Laplacians, providing a direct pathway to solve the heat equation and other partial differential equations in fluid dynamics.

We bridge theory and execution by compiling these fault-tolerant protocols using deterministic „Repeat-Until-Success" logic, complete with rigorous resource estimation (gate counts, circuit depth, and qubit scaling).

The future of Quantum Linear Algebra is here, and it is Qrisp. Eclipse Qrisp.

Matic Petrič is a quantum researcher at Fraunhofer FOKUS and a contributor to Eclipse Qrisp. Holding a Master's from the University of Ljubljana, he develops high-level abstractions to bypass gate-level bottlenecks. Currently, he co-leads the development of Qrisp's BlockEncoding class, utilizing (G)QSP and (G)QSVT to reframe computation as polynomial transformations. His research applies Chebyshev approximations to eigenstate filtering, Hamiltonian simulation, and quantum linear systems. A seasoned speaker, Matic has shared his expertise at the WeAreDevelopers World Congress, making advanced quantum linear algebra accessible to the research community.

Contact: matic.petric@fokus.fraunhofer.de

Block Encoding Linear Combinations of Pauli Strings Using the Stabilizer Formalism | Niclas Schillo, Fraunhofer IAO / flaQship

The Quantum Singular Value Transformation (QSVT) is a powerful framework that promises quantum speedups for a broad class of problems, with performance critically determined by the cost of the underlying block encodings. In this work, we present a new method to construct quantum circuits that block encode linear combinations of Pauli strings. Our approach has two main ingredients: we first transform the Pauli strings into a pairwise anti-commuting set, making the resulting linear combination unitary and directly implementable as a quantum circuit; we then apply a stabilizer-based correction using an ancilla register to restore the original Pauli strings. The scheme requires only a logarithmic number of ancilla qubits in the number of Pauli strings, and can be generalized to larger ancilla registers to further reduce overall circuit complexity. Using numerical simulations, we compare our construction to the standard Linear Combination of Unitaries (LCU) approach and find comparable overall circuit complexity, with improved T-gate counts and potential advantages in circuit depth when exploiting structure in the target operators.

Niclas Schillo is a quantum computing researcher at the Fraunhofer Institute for Industrial Engineering IAO and the Institute of Industrial Engineering and Technology Management (IAT) at the University of Stuttgart, where he works on quantum simulation algorithms and industrial applications of quantum computing. He is also a PhD student at the University of Freiburg, focusing on quantum simulation algorithms with a focus on block-encoding techniques.

Contact: niclas.schillo@iao.fraunhofer.de

Building resource-efficient Block-Encodings for Quantum Simulations | Leon Rullkötter, Fraunhofer IAO / flaQship

The construction of efficiently implementable block-encoding operators is essential for Quantum Signal Processing-based quantum algorithms, for example Hamiltonian simulation. State-of-the-art methods are well-suited for sparse and highly structured matrices but often suffer from intense resource requirements and a bad subnormalization for dense, unstructured inputs. We have developed a two-step method for block-encoding complex Hamiltonians with improved gate complexity, ancilla overhead, and subnormalization. First, the Hamiltonian is partitioned into subsystems of up to 10–15 qubits which are block-encoded separately using variationally compiled parameterized quantum circuits that are constructed classically. By adjusting the quantum circuit to the target submatrix, the number of parameterized gates can be closely matched to the degrees of freedom of the target using only a single ancilla qubit.The ansatz can also be symmetrized to constrain the circuit to specific subspaces, reducing resource requirements.
Second, the block-encoded partitions are composed into the full Hamiltonian via tensor products and linear combinations of block-encodings. Our method is most effective for Hamiltonians that partition/factorize into dense, low-structure submatrices. In these regimes, T-gate and two-qubit gate counts are an order of magnitude below competing methods such as Pauli-string LCU, accompanied by a subnormalization and ancilla count that scales with the number of partitions rather than the number of Pauli strings. We benchmark our approach on various different physical systems ranging from Heisenberg spin systems, over Fermi–Hubbard models, to ab-initio Hamiltonians from quantum chemistry.

Leon Rullkoetter is a research scientist at the Fraunhofer IAO in the quantum computing team. He studied physics at the University of Stuttgart, earning his Masters degree with a thesis focused on encoding Hamiltonians into quantum circuits using a variational compilation of block-encodings and their benchmark in QSP-based Hamiltonian simulation quantum algorithms. During his time at Fraunhofer, he has further improved upon the previously developed block-encoding methods for a wider range of physical systems. Beyond that, he has worked on quantum optimization algorithms and is leading the quantum computing training program at the Fraunhofer IAO.

Contact: leon.rullkoetter@iao.fraunhofer.de

Development of a compact and dynamic ansatz for enhanced quantum efficiency | Dipanjali Halder, Technical University of Denmark

Predicting the physical and chemical properties of molecular systems fundamentally requires understanding electron behavior. While quantum mechanics provides a rigorous framework for electronic structure, obtaining solutions that are both accurate and computationally feasible remains a longstanding challenge. Conventional electronic structure methods are inherently limited by the exponential scaling of the Hilbert space with system size. In contrast, quantum computers can encode the same exponentially large Hilbert space using only a linear number of qubits, N, thus, offering a fundamentally more scalable alternative. However, current quantum devices are noisy and limited in qubit count, coherence time, and gate fidelity, restricting the depth and complexity of implementable algorithms. This necessitates the development of resource-efficient quantum chemistry methods tailored to near-term hardware.
In this context, my work focuses on simulating molecular systems using quantum computing paradigms. Among proposed approaches, the Variational Quantum Eigensolver (VQE) is particularly promising for NISQ devices. Its performance, however, depends critically on the choice of ansatz. Chemically inspired ansätze can be accurate but often involve high gate depth and complex parameter spaces that hinder optimization.
To address this, we developed a chemically motivated dual-exponential coupled-cluster ansatz that captures higher-order excitation effects through low-rank parametrizations within VQE. Additionally, we introduced a first-principles-based dynamic approach that adapts to system-specific chemistry while eliminating the need for pre-circuit or gradient evaluations, enabling efficient and accurate ground-state simulations of many-electron systems.

Dipanjali Helder is a quantum computing researcher specializing in hybrid quantum-classical algorithms for quantum chemistry. Currently a Postdoctoral Researcher at the Technical University of Denmark, she focusses on development of scalable, noise-resilient methods for molecular simulation compatible with near-term quantum hardware. She earned her Ph.D. from the Indian Institute of Technology Bombay and has collaborated with IBM Quantum on implementing and benchmarking algorithms on real devices. Her work focuses on variational algorithms and chemically inspired ansätze, aiming to enable practical quantum advantage in molecular and materials simulations.

Contact: dipha@kemi.dtu.dk

Discovering Logical Operations for Arbitrary Quantum Error Correction Codes with Machine Learning | Dr. Daniel Scherer, Fraunhofer IIS

Quantum error correction and fault tolerance are essential for the reliable operation of quantum computers, as near-term hardware remains highly susceptible to noise from decoherence and control imperfections. Prior work has shown that machine learning can be used to tailor quantum error correction codes to specific noise structures and reduce qubit overhead versus established stabilizer codes. We extend this idea from memory protection to computation with a variational procedure that learns fault-tolerant logical operations for arbitrary additive and non-additive codes, termed Variational Early Fault-Tolerant Quantum Computing (VarEFTQC).

This is realized by minimizing a fidelity-based loss that aligns target logical channels with learned implementations, with trainability supported by regularization techniques that remove local minima from the loss landscape. By shaping the ansatz to enforce diverse notions of transversality, the resulting logical primitives are inherently constructed to guarantee fault tolerance. We validate the approach by re-learning logical operations for established stabilizer codes. Furthermore, we demonstrate the possibility of jointly learning noise-tailored encoders and their logical gate sets. We also analyze the concatenation of learned codes, observing up to two orders of magnitude overhead reduction under structured noise.

Finally, we show that VarEFTQC discovers noise-tailored codes supporting a transversal gateset for IQP circuit families. Because key expectation values are efficiently estimable while sampling remains hard under reasonable assumptions, these circuits are promising for quantum generative models, with potential applications in molecular and materials design.

Daniel Scherer is a theoretical physicist working at the intersection of quantum computing, algorithms, and software and head of the Quantum Compilation research group at Fraunhofer IIS in Nuremberg, Germany. His research focuses on the compilation layer of the quantum software stack, with an emphasis on scalable quantum computation through circuit cutting (near-term), distributed quantum computing (fault-tolerant), machine-learning–based quantum circuit optimization, quantum circuit synthesis, and resource efficient quantum error correction. His academic trajectory spans condensed matter theory, quantum algorithms, and software for quantum computers, with a strong emphasis on developing techniques that improve efficiency, robustness, and scalability across heterogeneous quantum hardware platforms.

Contact: daniel.scherer2@iis.fraunhofer.de

Efficient Calculation of Green's Function from Time-Evolution with Classical Signal Processing | Dr. Jannis Ehrlich, Fraunhofer IWM

Single-particle Green's functions are central objects in many-electron systems encoding spectral and essential single-particle properties. Quantum computers offer a natural framework for their efficient evaluation through their direct simulation. In this work, we investigate a time-evolution-based approach to computing Green's functions that is designed for the early and full fault-tolerant era of quantum computing. We demonstrate how relevant information can be extracted from real-time data using classical signal-processing techniques, enabling the reconstruction of spectral functions even from noisy simulations. Furthermore, we analyse the requirements on hardware quality to obtain reliable results.

Jannis Ehrlich is a physicist and mathematician with a strong background in theoretical and computational science. He studied physics and mathematics at the University of Bremen, where he developed a deep interest in quantum systems. Pursuing this passion, he moved to Aachen to complete his PhD, focusing on method development for correlated electron systems. Since 2021, Ehrlich has been serving as the lead scientific researcher for quantum algorithms for material simulation at the Fraunhofer Institute for Mechanics of Materials. His work bridges quantum computing and materials science, aiming to revolutionize how we model and predict the behavior of functional materials.

Contact: jannis.ehrlich@iwm.fraunhofer.de

Efficient Spin-Adapted Initial State Preparation for Quantum Computing | Hampus Brunander, CASUS/ HZDR

The performance of quantum algorithms for strongly correlated electronic systems relies on the overlap between the initial trial wavefunction and the ground state. Since the cost of state preparation must not outweigh the overlap improvement nor be more than a fraction of the total algorithm's cost, we identify regimes where spin-adapted wavefunctions implemented with a shallow circuit yield high overlaps. By adapting classical spin-group approaches, we use Localized Orbitals to identify the optimal spin-coupling ordering. This chemically motivated approach constructs a spin-adapted state that provides high overlap with a hardware-efficient implementation. We demonstrate that this strategy significantly improves fidelity for challenging systems, such as the stretched nitrogen dimer and iron-sulfur clusters.

Hampus Brunander holds a BSc in Chemical Engineering with Engineering Physics and an MSc in Nanotechnology from Chalmers University of Technology. He currently pursues a PhD in quantum computing for quantum chemistry at CASUS/HZDR in the AI4Quantum group. His research focuses on spin-adapted approaches for strongly correlated systems under the supervision of Prof. Thomas Kühne and Dr. Werner Dobrautz.

Contact: h.brunander@hzdr.de

Exploring Quantum Annealing for Coarse Grained Protein Folding | Timon Scheiber, Fraunhofer IGD

The protein structure prediction problem has wide spread applicability to many aspects of modern drug development. We explore the potential application of quantum annealing to address the protein structure problem (PSP). To this end, we compare several proposed ab initio protein folding models for quantum computers and analyze their scaling and performance for classical and quantum heuristics. Furthermore, we introduce a novel encoding of coordinate based models on the tetrahedral lattice, based on interleaved grids. Our findings reveal significant variations in model performance, with one model yielding unphysical configurations within the feasible solution space. Furthermore, we conclude that current quantum annealing hardware is not yet suited for tackling problems beyond a proof-of-concept size, primarily due to challenges in the embedding. Nonetheless, we observe a scaling advantage over our in-house simulated annealing implementation, which, however, is only noticeable when comparing performance on the embedded problems.

Timon Scheiber is an early career researcher, currently employed at the Fraunhofer Institute for Graphical Data Processing (IGD). Since the earlier days of his career he has a fascination for quantum mechanics and graduated from TU Darmstadt with a focus on theoretical quantum theory (Bachelor's) and experimental quantum computing with neutral atoms (Master's).
His current area of research focuses on quantum computing applications in the noisy intermediate quantum era and beyond. Based on his obtained insights Timon hopes to branch out into fault tolerant algorithms, which rapidly seem to be coming within reach.

Contact: timon.florian.scheiber@igd.fraunhofer.de

Material simulation by post-processing DFT calculations | Erik Schultheis, German Aerospace Center (DLR)

Quantum chemistry and material simulation are one of the most promising applications of quantum computers. Studying the ground and excited states of these systems with quantum computers requires a Hamiltonian describing the system.

We present a framework which generates many-body Hamiltonians for periodic crystal structures using Kohn-Sham orbitals from plane-wave density functional theory calculations performed with Quantum ESPRESSO. This Hamiltonian can be solved with classical algorithms, e.g. exact solvers, or using quantum algorithms. For strongly-correlated systems, where DFT struggles to give reliable results, we expect that our workflow in combination with (fault-tolerant) quantum computing is used to perform more accurate simulations of material systems.

We demonstrate our framework by investigating partial atomic charges in crystal structures using Bader charges computed from ground-states estimated using VQE. Bader charges are charges assigned to each atom in the computational cell of the crystal and provide insights in, e.g., bonding between atoms, charge-transfer, or oxidation states. Besides that, we are able to calculate excited states and material properties that can be calculated from ground and excited state energies. Further, we can also perform geometry optimization of the simulated material structures using analytical gradients.
Since we need (early) fault-tolerant quantum computers and suitable quantum algorithms that are able to find ground and excited states of these systems, this symposium is the perfect place to exchange ideas, discuss applications and build a path for using quantum computers to simulate materials.

After his bachelor and master studies in physics **Erik Schultheis** is currently in his fourth year of a PhD at the German Aerospace Center (DLR) in Cologne under the supervision of Prof. Jakob Kottmann from the University of Augsburg. His research focuses on bridging the gap between classical density functional theory (DFT) simulations of materials and quantum computing. This involves developing a workflow that connects DFT results with quantum computing, as well as algorithm research for performing electronic structure calculations using quantum circuits composed of (fermionic) excitations.

Contact: erik.schultheis@dlr.de

Neural Quantum States and DMRG for Similarity-Transformed Systems | Mohammed Boky, TU Dresden/ScaDS.AI

Similarity transformations have proven to be useful techniques for reducing computational costs while accurately extracting the ground state energy of quantum many-body and quantum-chemistry systems. Although applying this transformation leads to the Hamiltonian becoming non-Hermitian, its eigenspectrum remains unchanged. This non-Hermiticity does yield distinct left and right eigenvectors that form a biorthogonal system. In this work, we investigate the effective differences and practical challenges of optimizing computational methods for these distinct left and right eigenstates. Focusing on similarity-transformed quantum many-body systems such as the transverse-field Ising model, we investigate two computational approaches: the Density Matrix Renormalization Group (DMRG) and Neural Quantum States (NQS). We evaluate how the choice of targeting the left or right eigenvector impacts the optimization, convergence, and computational complexity of these approaches and compare these against their biorthogonal counterparts.

Mohammed Boky is a first year PhD student at ScaDS.AI (Center for Scalable Data Analytics and Artificial Intelligence) hosted at TU Dresden in the AI4Quantum group led by Dr. Dobrautz. His work mainly focuses on method development with the main interest being neural quantum states and non-hermitian optimization. The systems he likes to target with these techniques are mainly quantum many-body and quantum chemistry systems.

Contact: mohammed.boky@tu-dresden.de

Noise Resilience and Robust Convergence Guarantees for the Variational Quantum Eigensolver | Mirko Legnini, University of Stuttgart

Variational Quantum Algorithms (VQAs) are a class of hybrid quantum-classical algorithms that leverage on classical optimization tools to find the optimal parameters for a parameterized quantum circuit. One relevant application of VQAs is the Variational Quantum Eigensolver (VQE), which aims at steering the output of the quantum circuit to the ground state of a certain Hamiltonian. VQEs cover a wide range of applications in quantum natural sciences, including ground state preparation in quantum chemistry and quantum simulation. Over the last few years, significant research effort has been devolved to characterize the optimization landscape of such problems. In particular, relevant problems include the characterization of singular points and convergence guarantees.
In the interest of robustness, we focus on tackling such problems when an ideal VQA is affected by noise, both coherent and decoherent. We provide upper bounds for the distance between the perturbed and the ideal optimal parameters. Furthermore, we derive convergence guarantees for perturbed VQAs. Last, we address the specific case of depolarizing noise and coherent control errors. Our results are supported by numerical simulations implemented via Pennylane.

Mirko Legnini received his B.Sc. in Computer Science in 2022 and his M.Sc. in Automation Engineering in 2025 at the University of Bologna. He is currently a researcher at the Institute for Systems Theory and Automatic Control at the University of Stuttgart, a position he has held since May 2025. His research interests focus on variational quantum computing and system theoretical properties of optimization algorithms.

Contact: mirko.legnini@ist.uni-stuttgart.de

Optimisation of Partially Fault-Tolerant Quantum Computation in Neutral Atoms | Stefano Veroni, University of Oxford

To reduce the currently prohibitive overhead of fully fault-tolerant (FT) universal computation, the framework of partial fault-tolerance has recently been proposed.
While Clifford gates remain fully FT, arbitrary-angle rotations are natively implemented, rather than synthesised, at the expense of reduced resilience against specific protocol-dependent faults.
While this „Space-Time efficient Analog Rotation" (STAR) architecture offers a potential orders-of-magnitude reduction in the cost of universal computation, its practicality depends on accurate noise modelling and hardware co-design.
Our work rigorously characterises and further optimises the protocol's performance, with a focus on neutral atom architectures.
These are among the most promising platforms for digital computation, offering large scalability, high-fidelity operations, mid-circuit measurements, and non-local connectivity, as well as reduced error-correction overhead by means of 'algorithmic' fault-tolerance.
Our contributions are threefold. First, we improve the accuracy in the modelling of the protocol's noise, better informing subsequent design choices.
Second, we develop a numerical method to exactly estimate the scheme's performance, despite its non-Clifford nature, within sampling deviations.
Third, addressing the architecture's critical sensitivity to specific hardware faults, we perform pulse-level optimization of two-qubit Rydberg gates, and ab initio calculations of their error channel.
Altogether, these results validate the partially FT architecture for near-term universal computation, open new prospects on its resilience and scalability, and present a full-stack framework for robust quantum computation.

Stefano Veroni is a 2nd year PhD student at the University of Oxford, where he works in Prof Daley's Theory of Quantum Systems group.
His research focuses on estimating the effects of noise in neutral-atom quantum computers, and tailoring gate-optimisation and error-correction techniques to suppress them.
Previously, he has worked for one year on similar topics in Munich's startup planqc GmbH, which focuses on developing digital neutral-atom devices.

Contact: stefano.veroni@physics.ox.ac.uk

QLDPC Codes on a Two-Dimensional Tweezer Array with Adjustable Columns | Fernando Lima, Fraunhofer IAO / flaQship

Fault-tolerant quantum computation requires robust protection against physical noise. Quantum error correction (QEC) provides this by encoding logical qubits redundantly into many physical qubits. Surface and color codes are attractive near-term QEC scheme candidates due to their high error thresholds and locally measurable stabilizers. However, both families encode only a constant number of logical qubits regardless of code size. Quantum LDPC (QLDPC) codes overcome this limitation by achieving high, constant encoding rates while retaining sparse, low-weight stabilizers. Their primary challenge is the non-local connectivity that their check structure demands. Neutral atom quantum computers are ideally suited to this challenge, offering reconfigurable qubit arrangements, long coherence times, and tunable long-range interactions via Rydberg excitations. On this poster, we present a QLDPC code construction framework tailored to a 20×100 tweezer array with independently adjustable columns, which provides a hardware-native mechanism to relax connectivity constraints. By designing error correction rounds as alternating sequences of stabilizer measurements and controlled column shifts, the non-local check structure of QLDPC codes is mapped directly onto the machine's native operations. A systematic code design tool is introduced that jointly enforces hardware connectivity constraints and the mathematical requirements of the target codes, enabling principled exploration of the available code space. The resulting codes are benchmarked via circuit-level simulation with realistic noise models and state-of-the-art decoders, demonstrating the viability of high-rate QLDPC codes on near-term neutral atom hardware.

Fernando Lima is a Scientific Researcher in the Quantum Computing team at Fraunhofer IAO. His research focuses on the topic of Quantum Error Correction, with particular interest in Fault Tolerant Quantum Computing and quantum Low-Density Parity Check codes (qLDPC). His experience consists of research and development on topics such as quantum compilation, stabilizer formalism, and quantum error correction, and his current work aims to contribute to the improvement of fault-tolerant quantum computing, specifically via qLDPC encoding on neutral-atom machines.

Contact: fernando.lima@iao.fraunhofer.de

Quantum channel polynomial processing | Tianhan Liu, IQM

We have implemented quantum signal processing procedure with a quantum channel, which we named as quantum channel polynomial processing. In this algorithm, one has the choice to compile Hamiltonian terms either through sampling or through LCU type of circuits, which allows for a NISQ implementation of the generation of a polynomial of a Hamiltonian. We have also implemented and run this algorithm on the IQM QPU for the finding of ground state energy for a couple of molecules.

Tianhan Liu received his Ph.D trainings in UPMC and Ecole polytechnique before doing couple of years of postdoc in the U.K., after which I have been working with IQM for the last five years.

Contact: tianhanliu@gmail.com

Quantum Feature Selection in Medical Data: LR-QAOA with Parity Twine Networks for Hardware-Aware Optimization | Mareike Garreis, Fraunhofer IAF

We apply a recently introduced version of the Quantum Approximate Optimization Algorithm using linear-ramp schedules (LR-QAOA) to the use-case of feature selection in medical data. Using a dataset from studies of dementia, we illustrate how quantum computing could be useful in medical diagnostics. Starting with the quantum formulation of the underlying quadratic unconstrained binary optimization (QUBO) problem, we highlight the principal challenges and recent methodological advances for deploying quantum-optimized feature-selection pipelines. When solving QUBO problems with the QAOA algorithm, a trade-off needs to be found between low circuit depth and convergence to the optimal solution with high probability. To address circuit-depth limitations inherent to near-term quantum hardware, we encode the circuit with parity twine networks, which allow for a higher number of optimization layers while keeping resource demands tractable. We also discuss how to optimize the circuit parameters without prior knowledge of the optimal solution of the optimization problem. Results from simulations with and without gate errors as well as measurement shot noise, and initial implementations on real hardware will be presented.

Mareike Garreis started her physics studies at the University of Freiburg in October 2020, including a year at Imperial College London (2022–2023). She completed her bachelor's degree in March 2024 and has since been pursuing a master's degree in Quantum Physics. Since November 2025, She has been working on her master's thesis, exploring quantum-inspired approaches to machine learning for medical diagnostics.

Contact: mareike.garreis@iaf.fraunhofer.de

Quantum Simulation of Magnetic Materials | Pascal Stadler, HQS Quantum Simulations

Quantum computers are increasingly accessible, yet demonstrations of physically meaningful simulations for real materials remain scarce. In our work we simulate low-energy magnetic excitations, specifically magnon spectra, of chromium tri-halide monolayers. Starting from ab-initio electronic structure calculations for these two-dimensional magnets, we derive an effective spin model and simulate low-energy spin excitations using a real-time propagation of the spin system on the commercial quantum computing cloud platform IQM Resonance. The results for up to 48 qubits are validated against classical benchmarks. While some spectral features remain challenging for today's NISQ devices, our simulation achieves good agreement at quasi-constant wall-time scaling, compared to the exponential scaling of classical methods. Our results demonstrates that, even in the absence of quantum advantage, useful quantum simulations of real materials are becoming possible for domain experts via commercial cloud access.

Pascal Stadler is a Senior Expert at HQS Quantum Simulations, with extensive experience in quantum computing and the simulation of open quantum systems on real quantum hardware. His work sits at the intersection of quantum simulation and materials science, driving the development of practical tools to study complex quantum phenomena.

Contact: pascal.stadler@quantumsimulations.de

Quantum-Assisted Ghost Gutzwiller Ansatz | Dr. P.V. Sriluckshmy, IQM

The ghost Gutzwiller ansatz (gGut) embedding technique was shown to achieve comparable accuracy to the gold standard dynamical mean-field theory method in simulating real material properties, yet at a much lower computational cost. Despite that, gGut is limited by the algorithmic bottleneck of computing the density matrix of the underlying effective embedding model, a quantity which must be converged within a self-consistent embedding loop. We develop a hybrid quantum-classical gGut technique which computes the ground state properties of embedding Hamiltonians with the help of a quantum computer, using the sample-based quantum-selected configuration interaction (QSCI) algorithm. We study the applicability of SCI-based methods to the evaluation of the density of states for single-band Anderson impurity models within gGut and find that such ground states of interest become sufficiently sparse in the CI basis as the number of ghost orbitals is increased. Further, we investigate the performance of QSCI using local unitary cluster Jastrow (LUCJ) variational quantum states in combination with a circuit cutting technique, prepared on IQM's quantum hardware for system sizes of up to 11 ghost orbitals, equivalent to 24 qubits. We report converged gGut calculations which correctly capture the metal-to-insulator phase transition in the Fermi-Hubbard model on the Bethe lattice by using quantum samples to build an SCI basis with as little as 1% of the total CI states.

P.V. Sriluckshmy is a Senior Quantum Engineer, in the Algorithms and Error Control Department at IQM Quantum Computers in Germany. Her work is centered on developing hybrid quantum classical algorithms for Fermionic Simulation applications. Her research focus involves the in-depth study of condensed matter theory, particularly using embedding, perturbative, and mean-field approaches to solve Hubbard-type models. Her academic and research background includes affiliations with the Kings College London (KCL) in UK, Max Planck Institute for the Physics of Complex Systems (MPI-PKS) in Germany and The Institute of Mathematical Sciences (IMSc) in India.

Contact: pv.sriluckshmy@iqm.tech

Resource-efficient magic factories for arbitrary levels of the Clifford hierarchy | Christophe Goeller, ParityQC

Universal fault-tolerance can be achieved by supplementing Clifford operations with magic state distillation, with magic T state being the most popular choice. We introduce magic factories for noise bias qubits for efficient distillation of gates from kth level of the Clifford hierarchy using approximatively 2^{k+2} physical qubits. We provide constructive schemes for composing magic factories for an arbitrary level of the Clifford hierarchy. Our benchmarks demonstrate advantage of higher-level gate distillation over the (Clifford + T) gate set both in terms of logical gate fidelities and space-time resource cost in experimentally relevant regimes. The proposed scheme hence offers a promising building block for fault-tolerant architectures where small-angle rotations are produced directly rather than approximated using a (Clifford + T) set.

Christophe Goeller is a quantum error correction researcher at ParityQC, focusing on designing efficient protocol for logical computation as well as efficient quantum error correction code for platform with specific noise bias, such as cat qubits.

Contact: c.goeller@parityqc.com

Sample-Based Quantum Diagonalization of Similarity Transformed Hamiltonians for Strongly Correlated Systems | Emanuele Ricci, ScaDS.AI

Strongly correlated fermionic systems provide a fundamental benchmark for both classical and quantum computational methods, as their accurate description remains challenging due to the rapid growth of many-body Hilbert space and the complexity of correlation effects. In this work, we use the Hubbard model as a testbed to investigate the impact of the transcorrelated (TC) transformation on the structure of the many-body problem. The TC formulation preserves the exact spectrum while reshaping the determinant-space representation of the ground state, thereby modifying how correlation is distributed across the relevant configurations.
We combine this reformulation with Sample-Based Quantum Diagonalization (SQD), a quantum-classical framework in which a quantum device is used to sample configurations from a correlated ansatz, while the final eigenvalue problem is solved classically in the subspace spanned by the sampled determinants. We show that the TC approach can enhance SQD in two complementary ways: first, by improving the sampling step and making the resulting determinant pool more informative, and second, by reducing the size of the subspace required to achieve accurate ground-state estimates. Altogether, these results indicate that the transcorrelated formulation provides a promising route to more efficient ground-state estimation from sampled configurations in strongly correlated lattice models.

Emanuele Ricci is an early-stage PhD student at TU Dresden and ScaDS.AI, where he works on quantum algorithms for electronic structure and strongly correlated systems under the supervision of Dr. Werner Dobrautz. Before starting his PhD, he completed an internship at the Quantum Intelligence Lab in Milan under the supervision of Prof. Prati, which developed into his Master's thesis on a hybrid quantum–classical reservoir computing algorithm. After graduation, he continued with the same group for seven months as an external collaborator.

Contact: emanuele.ricci@tu-dresden.de

Simulating Electron Transfer: Noise is Fault Tolerant | Prof. Dr. Birger Horstmann, German Aerospace Center (DLR)

Simulating large electronic networks with vibrational environments is challenging due to long-lived vibronic excitations. Quantum computers offer a promising platform for modeling open quantum systems. We simulated an electron-transfer model with one donor and up to nine acceptors on IBM's superconducting quantum processor, using a model-specific error mitigation scheme. Our results with up to 20 qubits closely match classical calculations, revealing electronic and vibronic transfer resonances at expected driving forces. We conducted multiple experiments per system size to account for error fluctuations. Since vibronic transfer is entanglement-driven, this simulation benchmarks hardware capacity to generate and sustain entanglement, defined by the largest system size yielding accurate results.

Prof. Birger Horstmann studied Physics and Mathematics at the University of Jena and the University of Cambridge. He completed his PhD at the Max Planck Institute of Quantum Optics (MPQ), focusing on quantum information and open quantum systems. His research connects theoretical modeling with experiments. Currently, he is a group leader at the German Aerospace Center (DLR), studying battery chemistry with quantum chemistry and thermodynamic engineering.

Contact: birger.horstmann@dlr.de

Simulation of additive binding energies in asphalt using sample-based quantum diagonalization (SQD) | Marc Maußner, infoteam Software AG

2025 marks the UN International year of Quantum Science and Technology. Not only this, but also the fact that more and more useful - not only toy-sized - applications enter the industrial sector shows that this technology is on the leap from being emergent to entering and broadening in real world industry use cases.
It is proclaimed that the first domain to profit from this will be material and chemical simulation. We created a full workflow comprising as input industry relevant molecules, applying ML methods for geometry optimization and calculating the binding energy with an quantum (-inspired) approach. Afterwards our results are benchmarked against the classical DFT calculations.
We show with our approach that with current NISQ hardware also relevant calculations can be done.

Marc Maußner is Senior Consultant at infoteam Software AG, Germany. He is working as consultant in the fields of Functional Safety, Cybersecurity and Quantum Computing. He likes to work at the intersections of the domains resulting in combining Functional Safety and Cybersecurity requirements during product and project life cycle and Cybersecurity aspects in Quantum Computing, especially in Quantum Machine Learning. Beginning with Deloitte's Quantum Climate Challenge in 2023 he started to get curious about chemical simulations on quantum computers.

Contact: marc.maussner@infoteam.de

Towards battery simulations on quantum computers | Dr. Juliane Heitkämpfer, German Aerospace Center (DLR), Institute of Engineering Thermodynamics

Quantum computers hold significant promise for the efficient and accurate simulation of strongly correlated materials, including those critical to next-generation battery technologies. However, current quantum hardware is constrained by limited qubit counts and susceptibility to decoherence, making exact simulations of complex materials infeasible. In response, the Noisy Intermediate-Scale Quantum (NISQ) era has fostered the development of hybrid quantum-classical algorithms that can operate effectively within these limitations. In this work, we apply NISQ-compatible methods to investigate fundamental processes occurring inside battery systems, especially in organic electrode materials. A key aspect of our approach is the decomposition of these systems into active spaces; reduced regions that capture the most chemically relevant electrons and interactions. Within these active spaces, quantum algorithms are employed to resolve the electronic structure with high precision. By strategically focusing quantum computational resources where they are most impactful, our approach highlights the potential of quantum computing in advancing the fundamental understanding of battery materials, marking an early but significant step toward practical quantum simulations in energy storage research.

Juliane earned a B.Sc. and M.Sc. in Chemistry (Physical Chemistry) at the Karlsruhe Institute of Technology (KIT). She then pursued a Ph.D. in Theoretical Chemistry at the University of Stuttgart with the title "Computational Investigation of Catalytic Reaction Mechanisms".
Since August 2023 Juliane is a postdoctoral researcher at the Institute of Engineering Thermodynamics, German Aerospace Center (DLR), Ulm. The current focus is on simulating energy storage materials on quantum computers, complemented by classical atomistic modelling e.g. in collaboration with the DTU Energy Department in Copenhagen.

Contact: juliane.heitkaemper@dlr.de

Towards Real Chemistry Molecules with Valence Bond Theory for Quantum Computing | Francisco Javier del Arco Santos, University of Augsburg

Despite being presented as a promising application of Quantum Computing, most of the applications for chemistry have been demonstrated only on relatively small active spaces. This limitation reflects both the noise and constraints of current quantum hardware and the exponential scaling of classical methods. Many different approaches have been developed, which, in analogy to classical quantum chemistry methods, leverage the scaling by reducing the level of theory (accuracy) on arbitrary subspaces. However, it does not exist a cheap general automatic subspace selection routines, making it a task that already requires certain expertise.
In the presented work, we have started from our previous hybrid Fermionic-Bosonic encoding, which relies on restricting some subset of orbital occupancy. This leads to shallower circuits and a considerably reduced amount of non-commuting Hamiltonian terms. We then leverage the structured approach of Quantum Valence Bond Theory in order to rationalize the well-resolved space selection together with the circuit design. This way, we have been able to push the simulability barrier towards chemically relevant systems. Moreover, we present a NISQ compatible routine in order to move this approach towards the basis set limit.

Currently **Francisco Javier del Arco Santos** is a PhD student at the Chair of Quantum Algorithms of the University of Augsburg, working on quantum chemistry for quantum computing. Previously he carried his Bachelor in Chemistry on the University of Valencia of Spain, with a thesis on excited states chemistry. Then, he did his Master on Theoretical Chemistry and Computational Modelling on the Sorbonne University, Paris. Followed on an international stay on the KU Leuven, Belgium, for his master thesis on silica layer catalysis.

Contact: francisco.del.arco.santos@uni-a.de

Trade-offs Between Chemical Accuracy and Algorithmic Resources in Transcorrelated Quantum Chemistry | Cheng-Lin Hong, HZDR / CASUS

One of the major challenges in quantum chemistry on quantum computers is the large number of qubits required to achieve accurate results close to the complete basis set (CBS) limit. The transcorrelated (TC) method addresses this challenge by using a non-unitary similarity transformation to incorporate electron correlation effects directly into the Hamiltonian, thereby accelerating convergence toward the CBS limit and significantly reducing qubit overhead. A key complication is that the projected TC Hamiltonian is non-Hermitian and non-normal, which limits the direct applicability of standard Hermitian quantum algorithms and introduces eigenvector-sensitivity effects relevant to non-normal solvers.
For such non-normal operators, the complexity of several recent algorithms depends explicitly on the condition number. Understanding and estimating these condition numbers is therefore essential for assessing both algorithmic complexity and quantum resource requirements. In this work, we first study an exactly solvable model—the one-dimensional harmonic oscillator with a delta-function potential—to develop a systematic understanding of the transcorrelated method. Within this setting, we investigate two distinct one-parameter Jastrow factors and analyze their impact on two key aspects: (i) basis-set convergence and (ii) conditioning. We then extend the analysis to molecular systems to assess the practical implications of these findings in chemically relevant settings.

Cheng-Lin Hong holds a B.S. in Electrical Engineering and an M.S. in Theoretical Physics from National Taiwan University. He is currently a second-year PhD student at the Helmholtz-Zentrum Desden-Rossendorf (HZDR) within the Center of Advanced Systems Understanding (CASUS), advised by Werner Dobrautz. His research focuses on quantum information science and electronical structure simulations.

Contact: c.hong@hzdr.de

Impressum

The Fraunhofer Institute for Industrial Engineering IAO

Nobelstr. 12
70569 Stuttgart, Germany

is a constituent entity of the Fraunhofer-Gesellschaft, and as such has no separate legal status.

Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V.

Hansastraße 27 c
80686 München

Internet: www.fraunhofer.de

E-Mail: info@zv.fraunhofer.de

Responsible editors

Yeama Bangali
yeama.bangali@iao.fraunhofer.de

Chiara Stephan
chiara.stephan@iao.fraunhofer.de

Dr. Anne-Sophie Tombeil
anne-sophie.tombeil@iao.fraunhofer.de

Typesetting and Layout

Bianca Knülle

Image Credits: © Fraunhofer IAO

Supported by Dieter Schwarz Stiftung

HN FIZ Applied Quantum AI by Fraunhofer IAO & IPA

Fraunhofer HNFIZ

Fraunhofer Heilbronn Forschungs- und Innovationszentren HNFIZ

Learn more about the Fraunhofer Heilbronn Research and Innovation Center Applied Quantum AI.

https://flaqship.eu/

https://www.hnfiz.fraunhofer.de/en/services/applied-quantum-ai.html