Curriculum Vitae – Dr. Werner Dobrautz

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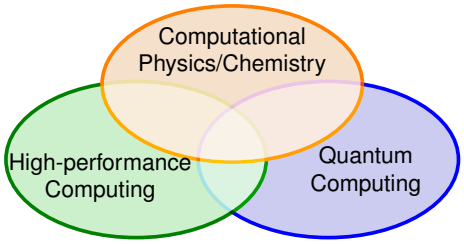

Personal Statement

After a graduate study of physics, with a specialization in **computational solid state physics**, and a subsequent Ph.D. in **theoretical/computational chemistry** in the field of stochastic wavefunction theory for **strongly correlated many-body problems**, I am currently an independent Marie Curie Postdoctoral Fellow and Group Leader at Chalmers University of Technology developing novel **quantum computing algorithms** to perform realistic *ab initio* electronic structure calculations on near-term quantum computing devices. I have strong knowledge of a variety of modern theoretical and **computational physics** and **chemistry** methods. As the main developer of the quantum Monte Carlo code `NECI`, I acquired extensive expertise in algorithm design and development in a **high-performance computing** environment.
The two main areas of my research are **(1)** the development of hybrid variational **quantum algorithms** and **error mitigation techniques** to accurately solve *ab initio* quantum chemistry problems on current quantum hardware, as well as **(2)** developing highly accurate **quantum Monte Carlo** methods for **high-performance computing** clusters to solve strongly correlated electron problems relevant to the green energy transition.

Professional and Academic Career

Since 7/2022	**Marie Skłodowska-Curie Postdoctoral Fellow** and **Group Leader**, Chalmers University of Technology and Wallenberg Centre for Quantum Technology, Gothenburg, Sweden Quantum algorithm development to enable accurate and efficient *ab initio* electronic structure calculations on current and near-term quantum computers
10/2021 – 6/2022	**Postdoc**, Chalmers University of Technology, Gothenburg and IBM Academic Network Development of novel quantum computing algorithms to perform realistic *ab initio* electronic structure calculations on near-term quantum computing devices
4/2019 – 9/2021	**Postdoc**, Max Planck Institute for Solid State Research, Stuttgart, Germany • Development of QMC methods for strongly correlated electron systems. Application to solid-state model Hamiltonians and strongly correlated bio-chemical transition-metal clusters. • Development of highly optimized massively parallel algorithms for HPC centers. • Collaboration with industry partners to enable accurate quantum chemical calculations on NISQ quantum computing devices.
9/2020 – 6/2021	**Math Teacher** at *Haus der Lebenschance*, eva e.V, Stuttgart, Germany Teaching math for adults attempting to catch up on graduation (6h / week)
10/2012 – 9/2014	**University Project Assistant**, Graz University of Technology, Graz, Austria Tutor in *Quantum Mechanics*, *Theoretical Electrodynamics*, *Advanced Quantum Mechanics* and *Advanced Computational Physics* and development of Monte Carlo methods for strongly correlated electron systems
10/2011 – 9/2012	**Data analyst** in the field of pharmaceutical process and product design, Research Center Pharmaceutical Engineering GmbH, Graz, Austria

Academic Studies

11/2014 – 3/2019	**Ph.D.** (Dr. rer. nat.) in theoretical quantum chemistry (*summa cum laude*), MPI for Solid State Research and University of Stuttgart, Germany, Ph.D. award date: 26.3.2019 Thesis: *Development of full configuration interaction quantum Monte Carlo (FCIQMC) methods for strongly correlated electron systems*, Supervisor: Prof. Ali Alavi
10/2011 – 3/2014	**MSc** (Dipl.-Ing.) in Technical Physics (*with distinction*), Graz University of Technology, Focus: Theoretical and Computational Physics, Graz, Austria, MSc award date: 28.3.2014
10/2007 – 4/2011	**BSc** in Technical Physics, Graz University of Technology, Graz, Austria

Career Breaks

2023 – 2024	**Parental Leave** – 6 months

Schools and Workshops

2023	**Lecturer** at Autumn School on *Applied Quantum Computing*, Oslo Metropolitan University
2023	**Lecturer** at *NordIQuEst Quantum Autumn School*, Gothenburg, Sweden
2022	**Lecturer** at Winter School in Theoretical Chemistry, *Quantum Computers for Chemistry*, University of Helsinki, Helsinki, Finland
2021	Quantum Open Source Foundation – QOSF – Mentorship Program
2021	Qiskit Global Summer School on Quantum Machine Learning
2019	Advanced C++ with Focus on Software Engineering, HLRS, Stuttgart, Germany
2017	European Summer School in Quantum Chemistry – ESQC, Sicily, Italy

Teaching, Pedagogical Experience and Supervision of Students

Lectures and Exercises

Year	Subject	Degree	Type	Week hours
2012-2013	Quantum Mechanics	2nd year BSc. Physics	Exercise	2
2013	Theoretical Electrodynamics	3rd year BSc. Physics	Exercise	2
2013	Advanced Quantum Mechanics	1st year MSc. Physics	Exercise	2
2013-2014	Advanced Computational Physics	2nd year MSc. Physics	Exercise	1
2020-2021	Math	Secondary School	Lec. & Ex.	6
2022, 2023	Quantum Simulation in *From quantum optics to quantum technologies* course	MSc./PhD Physics	Lecture	3 lectures
2022	*Quantum Computers for Chemistry*, Helsinki	Winterschool/PhD level	Lecture	3 lectures
2023	*Applied Quantum Computing*, Oslo	Autumnschool/PhD level	Lecture	2 lectures
2023	*NordIQuEst Quantum Autumn School*	Autumnschool/PhD level	Exercise	1 exercise

Pedagogical Training

2018	Workshop *Teaching during your PhD* at Graduate School of Stuttgart University
2022 – 2024	Currently obtaining the Swedish *Diploma in Teaching and Learning in Higher Education* as part of it completed the *University Teaching and Learning* course at Chalmers University

Supervision of students

2019 – 2021	Co-supervision of a Ph.D. student at the MPI Stuttgart
2021 – 2023	Co-supervision of a Ph.D. student at Chalmers University of Technology
2022	Supervision of two students in Physics Master course project *Building and programming a quantum computer* at Chalmers University
1/2023 – 6/2023	Supervision of a Master student at Chalmers University of Technology
1/2024 – 7/2024	Supervision of a Master student at Chalmers University of Technology
Since 9/2023	Supervision of a Ph.D. student at Chalmers University of Technology

Funding Acquisition

2022	223k EUR	Marie Skłodowska-Curie Postdoctoral Fellowship
2022	37k EUR	Funding for "*Frontiers of near-term quantum computing*" conference
2023	Contributed to the European Quantum Technology Flagship OpenSuperQPlus grant application	
2024	44k EUR	Vinnova – Attract, integrate and retain international excellence grant

Academic Service

2022 – 2023	Main organizer of the *Frontiers of near-term quantum computing* conference held in Gothenburg, August 2023, with 24 invited speakers and around 100 on-site attendees
2022 – now	Reviewer for *ACS Omega*, *Molecular Physics*, *Physical Chemistry Chemical Physics*, *The Journal of Physical Chemistry*, *Quantum*, *The Journal of Chemical Physics*, *npj Quantum Information*, *ACS Physical Chemistry Au*, *PRX Quantum, Physical Review A/Research*, *The Journal of Chemical Theory and Computation* and *The International Journal of Quantum Chemistry*
2022 – now	American Physical Society member
2023 – 2024	Committee member of the Quantum Computing paper track of the ISC High Performance 2024

Continuing Education, Leadership and Administrative Experience

2024	NaturalScience.Careers Workshop – *Introduction to leadership skills for scientists*
Since July 2023	**Young Investigator Group Preparation Program** at *Karlsruhe Institute of Technology* Preparation and Mentorship Program for Independent Group Leader Positions
2022 – 2023	Main organizer of the *Frontiers of near-term quantum computing* conference held in Gothenburg, August 2023, with 24 invited speakers and around 100 on-site attendees
2016 – 2021	Attended the MPI workshops on: *Building and managing your research group*, *Teaching during the PhD*, *Communication Skills*, and *Academic Leadership*
2015 – 2016	Ph.D. representative, MPI for Solid State Research and MPI for Intelligent Systems, Stuttgart, Germany. *Communicating information relevant to PhDs, organizing workshops, mentoring new Ph.D. students, organizing talks at the institute, and visits to scientific facilities in Europe.*

Invited Seminars:

2024	Fraunhofer IAO, QuantumBW Colloquium, Stuttgart Germany, *Quantum computing meets quantum chemistry: A potential new era of simulation and study*
2024	Quantinuum Ltd., Cambridge, UK, *Towards real chemical accuracy on current quantum hardware through the transcorrelated method*
2023	Algorithmiq Ltd., Helsinki, Finland, *Reducing necessary quantum hardware resources with explicitly correlated methods*
2021	IBM Research Zürich, Rüschlikon, Switzerland, *Reducing the computational footprint on quantum hardware by a correlated wavefunction Ansatz*
2020	Sorbonne University, Laboratoire de Chimie Theorique, Paris, France, *Non-unitary similarity transformation of the electronic Schrödinger equation via Gutzwiller and Jastrow factorization*
2020	King's College, Department of Physics, London, UK, *Non-unitary similarity transformation of the electronic Schrödinger equation via Gutzwiller and Jastrow factorization*

Conference Contributions – Talks:

2024	Faraday Discussions on Correlated electronic structure, London, *Reducing Quantum Circuit Depth for Noise-Resilient Quantum Chemistry using the Transcorrelated Method and Adaptive Ansätze*
2023	**Invited Talk**: QED-C Quantum talent showcase, online, *Towards real chemical accuracy on current quantum hardware through the transcorrelated method*
2023	**Invited Talk**: QVEST – Quo Vadis Electronic Structure Theory, Ringberg Castle, Germany, *Reducing necessary quantum hardware resources with explicitly correlated methods*
2023	**Invited Talk**: Chalmers SmallTalks, Chalmers University, Gothenburg, Sweden, *Chemistry Meets Quantum Computing: A New Era of Simulation and Study*
2023	APS March Meeting, Las Vegas, USA, *Accurate quantum chemistry calculations on near-term quantum computers enabled by the transcorrelated method*
2021	E-MRS Fall Meeting (Warsaw), *Spin-pure stochastic CASSCF applied to iron-sulfur clusters*
2021	**Invited Talk**: Quantum Bio·Inorganic Chemistry Society, online, *Spin-pure full configuration interaction Quantum Monte Carlo*
2021	**Invited Talk**: `OpenMolcas` Developers' eMeeting, Loughborough, UK (online), *Spin-pure Stochastic-CASSCF applied to iron-sulfur clusters*
2020	`OpenMolcas` Developers' eMeeting, Stuttgart, Germany (online), *Spin-pure Stochastic-CASSCF in OpenMolcas via spin-adapted FCIQMC*
2019	**Invited Talk**: `NECI` Developers Meeting, Stuttgart, Germany, *Application of the Transcorrelated Approach to the 2-D Hubbard Model*
2017	DPG Spring Meeting, *SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach*

Research-related Competences:

- **Computational Physics/Chemistry Software:** Expert knowledge of quantum Monte Carlo methods, esp. `NECI`. Well experienced with `PySCF` and `OpenMolcas`. Knowledge of `Molpro, iTensor, BlockDMRG, CASINO, TensorFlow, ALPS, Triqs` and `QuantumPackage`
- **Quantum Computing:** Expert knowledge of quantum algorithms development, expert knowledge of `Qiskit` and well-experienced with `PennyLane`.
- **Programming Languages:** Expert knowledge of `Fortran` and `Python`. Well-experienced with parallelization in an HPC setting with `OpenMP` and `MPI`. Knowledge of `C++`.
- **Development:** Expert knowledge of `Git` and experience with CI/CD workflows.