Curriculum Vitae – Dr. Werner Dobrautz

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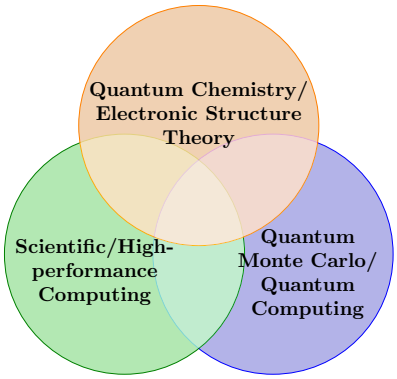

After a graduate study of physics, with specialization in computational solid state physics, and a subsequent Ph.D. in computational quantum chemistry in the field of stochastic wavefunction theory for strongly correlated electron systems, I am currently a Marie Skłodowska-Curie Postdoctoral Fellow at Chalmers University of Technology developing novel quantum computing algorithms to perform realistic *ab initio* calculations on near-term quantum computing devices. I have strong knowledge of a variety of modern theoretical and computational quantum chemistry methods and I acquired extensive algorithm design and development expertise as the main developer of the publicly available quantum Monte Carlo code `NECI` during my Ph.D. and consequent PostDoc.
The two main areas of my research are the **(1)** development of novel quantum computing algorithms to perform realistic *ab initio* calculations on near-term quantum computers as well as **(2)** developing highly accurate quantum Monte Carlo methods for high-performance computing clusters to solve strongly correlated electron problems.

Professional and Academic Research Experiences

Since 01.07.2023	**Remote Fellow – Young Investigator Group Preparation Program**, Karlsruhe Institute of Technology, Steinbuch Centre for Computing, Karlsruhe, Germany. Preparation and Mentorship Program for Independent Group Leader Funding Applications
Since 01.07.2022	**Marie Skłodowska-Curie Postdoctoral Fellow**, Chalmers University of Technology and Wallenberg Centre for Quantum Technology, Gothenburg, Sweden Quantum algorithm development to enable accurate and efficient *ab initio* calculations on current and near-term quantum computers
01.10.2021 – 30.06.2022	**Postdoc**, Chalmers University of Technology, Gothenburg and IBM Academic Network Development of novel quantum computing algorithms to perform realistic *ab initio* calculations on near-term quantum computing devices
01.04.2019 – 30.09.2021	**Postdoc**, Max Planck Institute for Solid State Research, Stuttgart, Germany • Development of highly accurate quantum Monte Carlo 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 high-performance computing centers. • Collaboration with industry partners to enable accurate quantum chemical calculations on NISQ quantum computing devices.
01.09.2020 – 30.06.2021	**Math Teacher** at *Haus der Lebenschance*, eva e.V, Stuttgart, Germany Teaching math for adults attempting to catch up on graduation (6h / week)
01.10.2012 – 30.09.2014	**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
01.10.2011 – 30.09.2012	**Data analyst** in the field of pharmaceutical process and product design, Research Center Pharmaceutical Engineering GmbH, Graz, Austria

Academic Studies

01.11.2014 – 26.03.2019	**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
01.10.2011 – 28.03.2014	**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
	Thesis: *Application of the FCIQMC algorithm to the two-dimensional fermionic Hubbard model*, Supervisor: Prof. Wolfgang von der Linden
01.10.2007 – 11.04.2011	**BSc** in Technical Physics, Graz University of Technology, Graz, Austria

Schools and Workshops

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
2017	Many Electron Collaboration Summer School of the *Simons Foundation*, Stony Brook University, New York, USA
2017	AWS Artificial Intelligence Bootcamp, Stuttgart, Germany
2015	Tensor Network Summer School, Ghent University, Belgium

Teaching, Pedagogical Experience and Supervision of Students

Supervision of students	
2021 – now	Co-supervision of a Ph.D. student at Chalmers University
2022	Supervision of two students in Physics Master course project *Building and programming a quantum computer* at Chalmers University
Jan. 2023 – June 2023	Supervision of a Master student at Chalmers University

Lectures

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 (Final Year)	Lecture & Exercise	6
2022	**Quantum Simulation** in *From quantum optics to quantum technologies* course	MSc./PhD Physics	Lecture	3 lectures
2022	**Quantum Computing for Quantum Chemistry**	Winterschool/PhD level	Lecture	3 lectures

Academic Service

2023 Co-organizer of Frontiers of near-term quantum computing workshop in Gothenburg, Sweden.

2023 Reviewer for *ACS Omega*, *Molecular Physics, Physical Chemistry Chemical Physics* and *International Journal of Quantum Chemistry*

Honors, Awards and Scholarships

2022 Marie Skłodowska-Curie Postdoctoral Fellowship

Invited Seminars

2023 Algorithmiq Ltd., Helsinki, Finland, *Reducing necessary quantum hardware resources with explicitly correlated methods*

2022 Max Planck Institute for Solid State Research, Stuttgart, Germany, *Reducing the computational footprint on quantum hardware by a correlated wavefunction Ansatz*

2021 IBM Research Zürich, Rüschlikon, Switzerland, *Reducing the computational footprint on quantum hardware by a correlated wavefunction Ansatz*

2020 Sorbonne Universités, 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*

2019 Vienna University of Technology, Department of Physics, Vienna, Austria, *Non-unitary similarity transformation of the electronic Schrödinger equation via Gutzwiller and Jastrow factorization*

Conference Contributions

Talks:

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 (virtual, Warsaw), *Spin-pure stochastic CASSCF applied to iron-sulfur clusters*

2021 Quantum Bio·Inorganic Chemistry Society, online, *Spin-pure full configuration interaction Quantum Monte Carlo*

2021 `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 `NECI` Developers Meeting, Stuttgart, Germany, *Application of the Transcorrelated Approach to the 2-D Hubbard Model*

2018 `NECI` Developers Meeting, Stuttgart, Germany, *Spin Symmetry and the Graphical Unitary Group Approach*

2017 DPG Spring Meeting, Dresden, *SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach*

Posters:

2023	APS March Meeting, Las Vegas, USA, *Reference-State Error Mitigation: A Strategy for High Accuracy Quantum Computation of Chemistry*
2022	A nano focus on quantum materials, Chalmers University of Technology, Gothenburg, Sweden, *Enabling Accurate Quantum Chemistry Calculations on Near-Term Quantum Devices*
2022	Science and Technology Day, Chalmers University of Technology, Gothenburg, Sweden, *Enabling Accurate Quantum Chemistry Calculations on Near-Term Quantum Devices*
2022	Wallenberg Centre for Quantum Technology Review Meeting, Gothenburg, Sweden, *Enabling Accurate Quantum Chemistry Calculations on Near-Term Quantum Devices*
2019	Congress of the International Society for Theoretical Chemical Physics, Tromsø, Norway, 2019, *The Transcorrelated Method in the Two-Dimensional repulsive Hubbard Model*
2019	Congress of the International Society for Theoretical Chemical Physics, Tromsø, Norway, 2019, *SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach*
2018	International Congress of Quantum Chemistry, Menton, France, 2018, *The Transcorrelated Method in the Two-Dimensional repulsive Hubbard Model*
2015	DPG Spring meeting, Berlin, 2015, *Efficient Implementation of SU(2) Symmetry using the Unitary Group in FCIQMC*

Personal Skills and Competences

Research Areas

- *Ab initio* Quantum Chemistry
- Quantum Computing
- Quantum Monte Carlo
- Method development
- Electronic Structure Theory
- Quantum Many-body physics
- Strongly Correlated Electron Systems
- Computational Solid State Physics

Research-related Competences

- **Computational 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.

Language Skills

- German (mother tongue)
- English (fluent)
- Swedish (basic)