

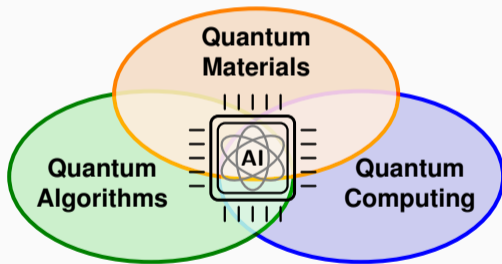
Research Group: AI 4 Quantum

Machine Learning for Quantum Simulation and Quantum Computing

Werner Dobrautz

CASUS Science Day 2024

DRESDEN
concept



INSTITUTE OF



PARTICIPATING INSTITUTIONS



FUNDED BY



My Background

PostDoc – **Quantum Computing**

Quantum Algorithms and Software
– **Error Mitigation** – **Electronic Structure** – **NISQ devices**



CHALMERS
UNIVERSITY OF TECHNOLOGY



Academic Network

WACQT | Wallenberg Centre for Quantum Technology

140M EUR Research effort for Sweden's Quantum Computer ≈30 PIs, 20 PostDocs and 40 PhDs



VINNOVA
Sweden's Innovation Agency

NordIQEst

HPC+QC ecosystem in the Nordics + Estonia
Lumi HPC + QAL9000 and Helmi QCs



OpenSuperQPlus

28 EU partners aiming to build a 1,000 qubit QC
Including a focus on HPC+QC integration

Quantum Materials

Quantum Algorithms

Quantum Computing



MAX PLANCK INSTITUTE
FOR SOLID STATE RESEARCH

PhD in **Computational Chemistry**

Quantum Chemistry – **Quantum Monte Carlo** –
HPC – **Strong Correlation** – **Transition Metals**

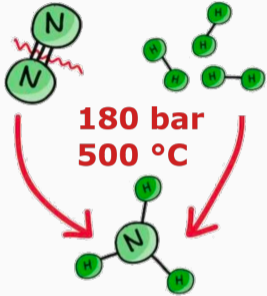


BSc/MSc Studies in **Physics**

Computational/Solid State Physics

Motivation: Haber-Bosch process and biological nitrogen fixation

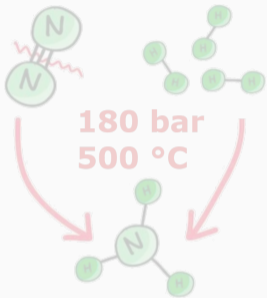
Haber-Bosch Process



- **Crucial for fertilizer production**
- 2% of world's energy consumption
- 3% of global carbon emissions
- 5% of natural gas consumption

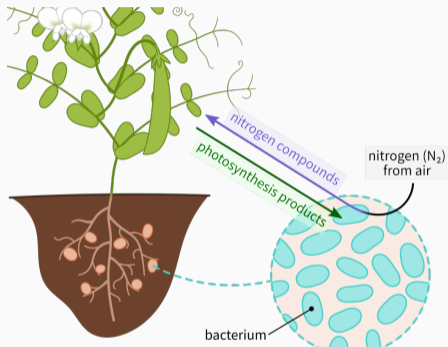
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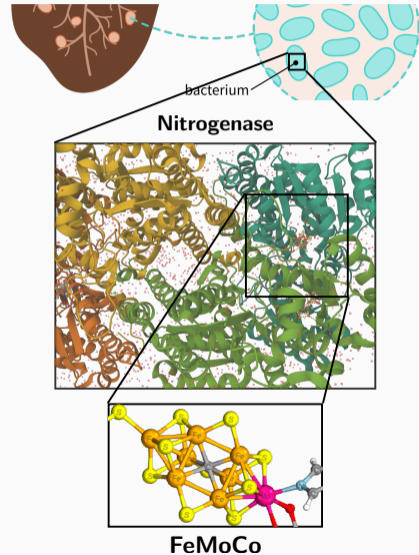
Biological nitrogen fixation



- **Ambient pressure and temperature**
- Not yet understood → Bio-catalysts for more efficient and greener ammonia production

Problem: Strongly correlated transition metal compounds

- **Transition metal clusters** act as catalysts: Iron-Molybdenum cofactor (FeMoCo) and other iron-sulfur clusters
- **Experimental study very difficult!**



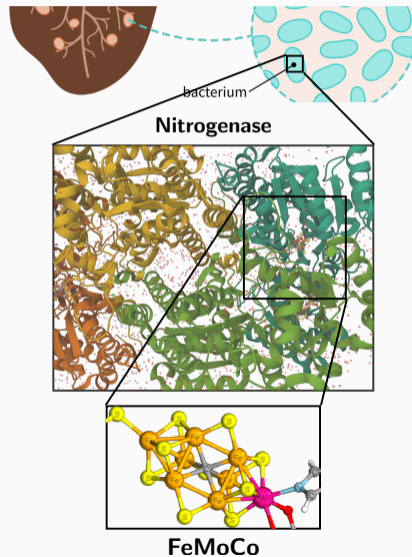
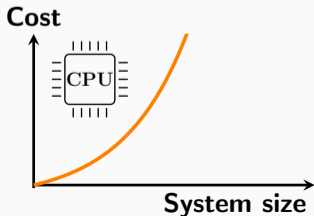
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- **Experimental study very difficult!**

→ Numerical studies of relevant quantum phenomena necessary → $\hat{H} |\Psi\rangle = E |\Psi\rangle$

We have the equations at hand, but **exponentially costly** on classical computers!



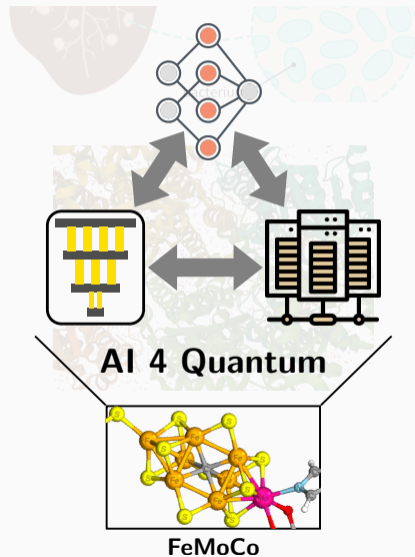
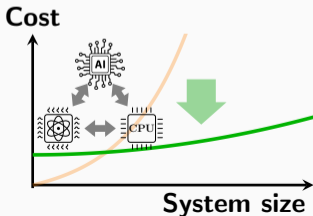
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Use a combined AI, HPC and QC approach for a potential computational speedup

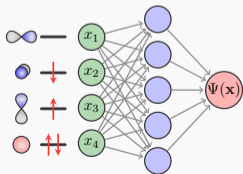


AI 4 Quantum

Synergistic AI+QC+HPC toolkit for the computational study of complex quantum matter

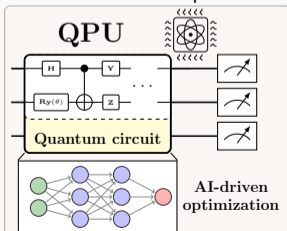
Neural Network States for Quantum Matter

- **Compress** exponential complexity of target solution, $\Psi(\mathbf{x})$
- **Resource reduction:** physics-informed, symmetry-preserving neural quantum states



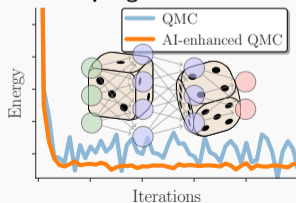
AI-driven Quantum Computing Approaches

- Increase **noise-resilience** and optimization of quantum algorithms
- **ML optimization** of quantum Ansätze: Gates and parameters



AI-enhanced Quantum Monte Carlo Methods

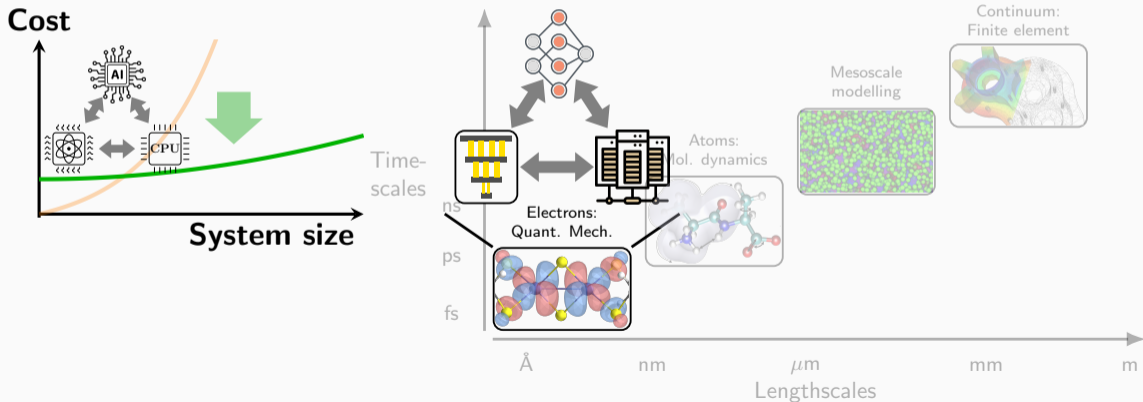
- **Extend reach** and acc. of QMC: AI-enhanced sampling of exponential state space
- Big data ML approach for **optimal sampling**



AI 4 Quantum – Overview

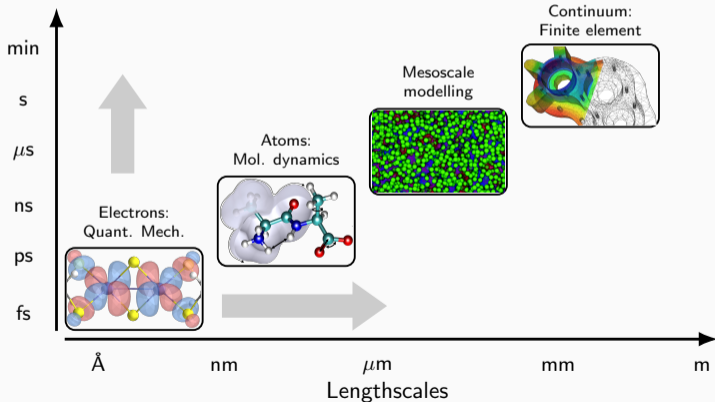
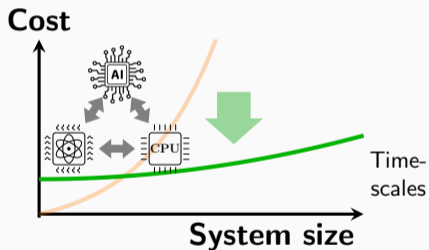
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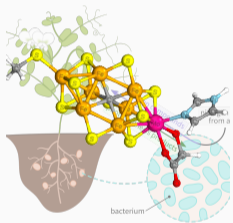
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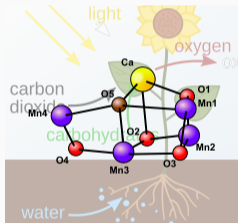


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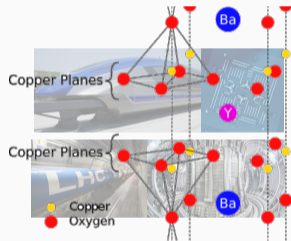
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Nitrogen fixation



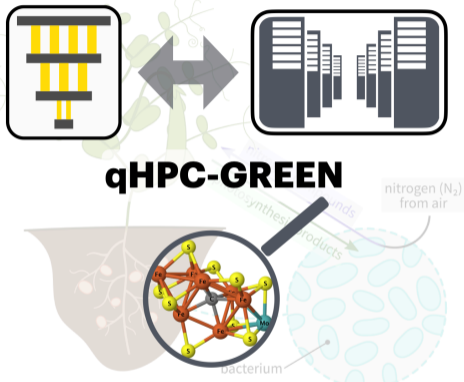
Artificial photosynthesis



High-T_c superconductivity

- Drug discovery
- Materials design
- Battery development
- ...

Long-term: applications for a wide-range of strongly correlated problems



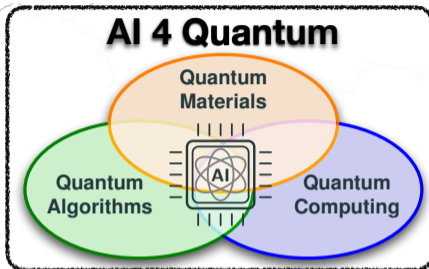
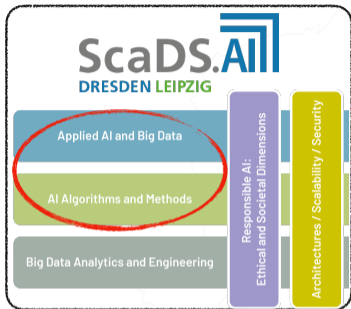
1.8M EUR

HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES
Helmholtz Investigator Group
1.5M EUR

5-year funding to establish JRG for developing QC+HPC methods to study quantum systems at the heart of biological nitrogen fixation



AI 4 Quantum's Fit and Added Value



HZDR
CASUS

- Fundamental phenomena of nature
- Matter under extreme conditions
- Understanding of complex systems
- Cangi, Kuc, Hecht, Bussmann, Dornheim, Kühne

TECHNISCHE UNIVERSITÄT DRESDEN

Research Priority Areas:

- Information Technology
- Energy, and Environment
- Materials Science

FACULTY OF COMPUTER SCIENCE
Modeling, Machine Learning, Simulation of Natural Systems

CIDS Center for Interdisciplinary Digital Sciences

CHAIR OF MATERIALS SCIENCE AND NANOTECHNOLOGY

DCMS **CHAIR OF THEORETICAL CHEMISTRY**

ct.qmat

DRESDEN concept

Scientific Area Committees:

- Information Technology & Microelectronics
- Materials & Structures

MPI-CPfS

IFW

Group



PhDs



PostDocs

I AM HIRING!

Physics, Chemistry, Computer Science,
Quantum Technology, AI / Machine Learning, ...

**Funding and
Acknowledgements**



Bundesministerium
für Bildung
und Forschung



SACHSEN

DRESDEN
concept



ScaDS.AI
DRESDEN LEIPZIG

HELMHOLTZ

HZDR



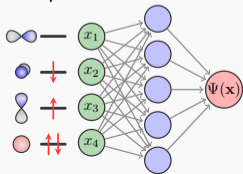
Thank you for your attention!

AI 4 Quantum

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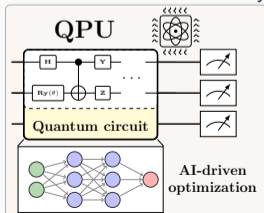
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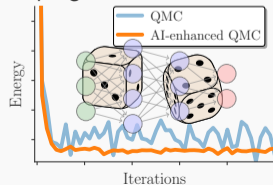
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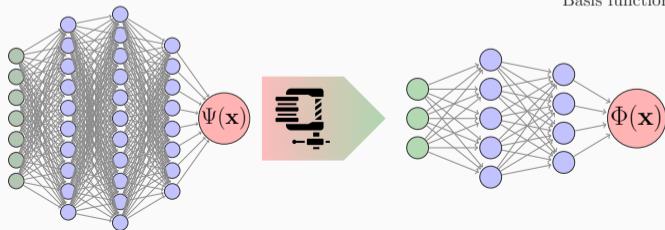
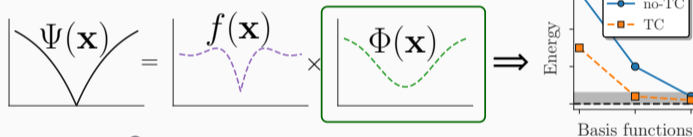
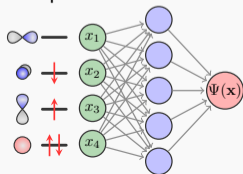
AI 4 Quantum – Details

AI 4 Quantum

Synergistic AI+QC+HPC toolkit for the computational study of complex quantum matter

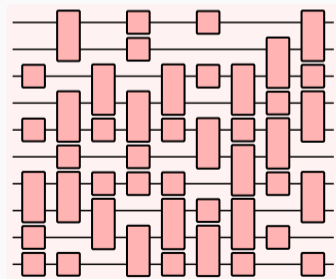
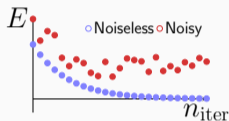
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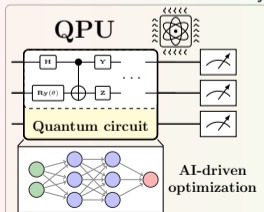
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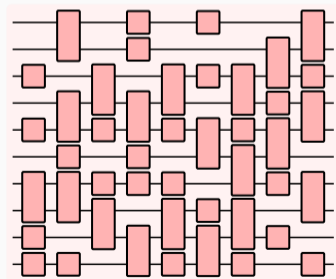
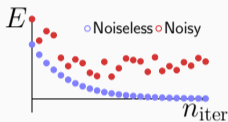
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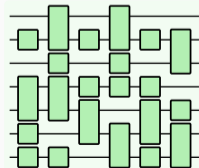
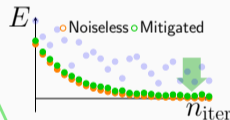
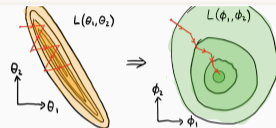
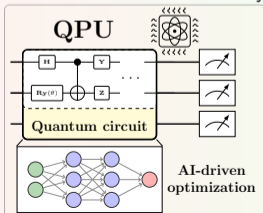
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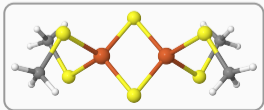
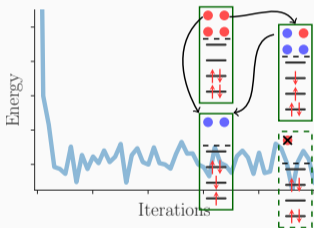
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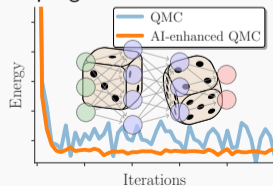
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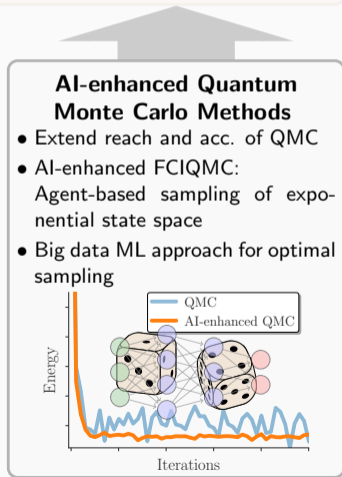
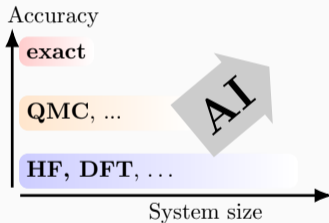
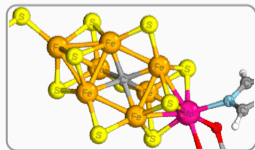
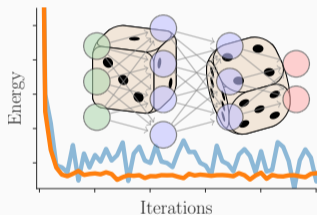
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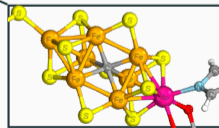
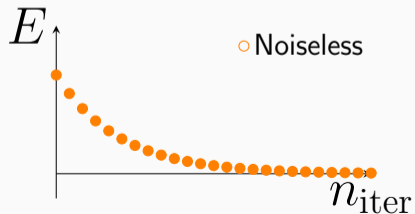
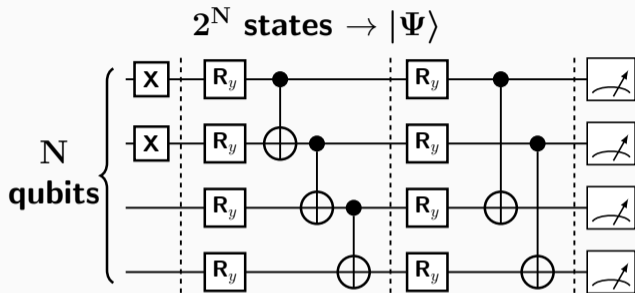
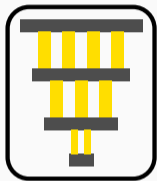
AI 4 Quantum – Details

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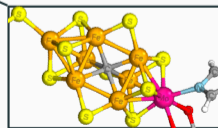
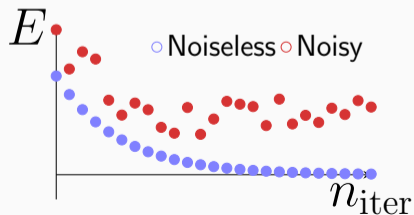
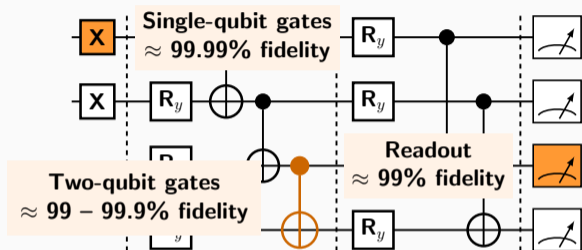
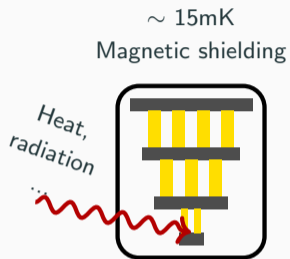
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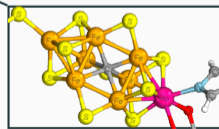
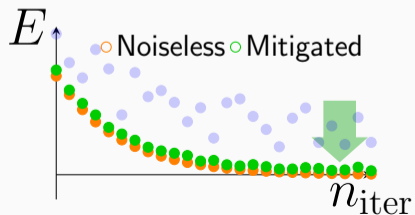
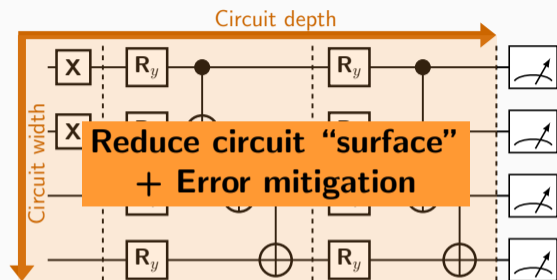
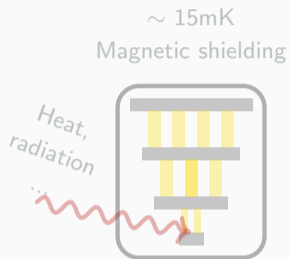
Problem: Noisy intermediate-scale quantum devices



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qHPC-GREEN – Overview

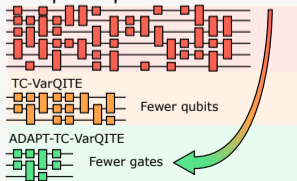
HPC+QC toolkit to study strongly correlated quantum chemistry problems

Simulation of bio-chemical transition metal compounds relevant for the **green energy transition**

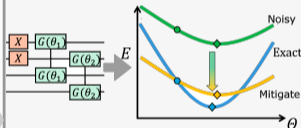
WP1

Resource reduction:

- Accurate calculations for relevant problems – Quantum imaginary time evolution
- Transcorrelation, active spaces, spin-symmetry and adaptive quantum Ansätze

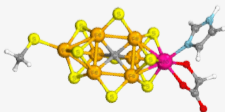


Error mitigation:



Relevant applications:

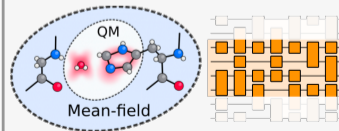
Electronic structure of transition metal complexes



WP2

Algorithms and software for relevant insights:

- Electronic properties
- Quantum embedding
- Excited states
- Efficient QC+HPC implementation



qHPC-GREEN – Overview

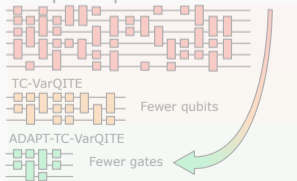
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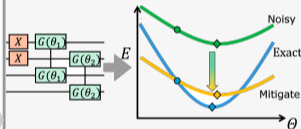
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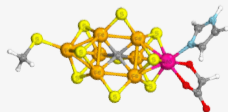
WP1-2

Error mitigation:



Relevant applications:

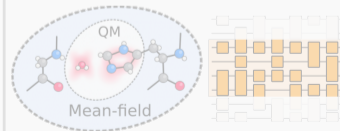
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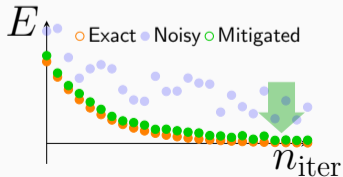
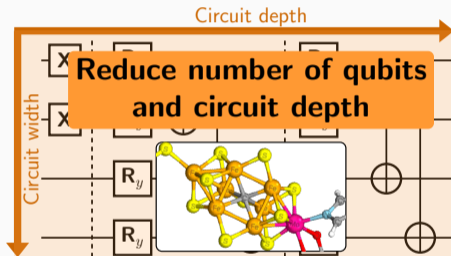
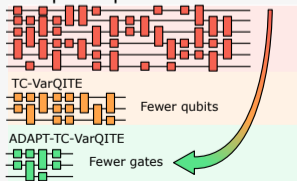
HPC+QC algorithms toolkit to study strongly correlated electron problems

Simulation of bio-chemical transition metal compounds relevant for the green energy transition

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Resource Reduction

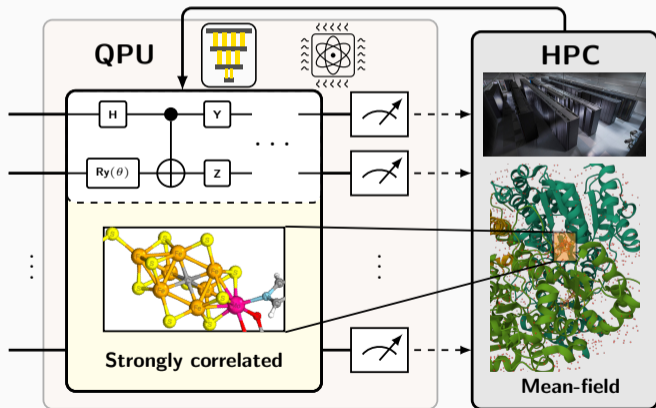
- Accurate calculations for relevant problems on current and future NISQ devices
- Transcorrelation, active spaces, spin-symmetry and adaptive quantum Ansätze



qHPC-GREEN – Overview

HPC+QC toolkit to study strongly correlated quantum chemistry problems

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- Electronic properties
- **Quantum embedding**
- Excited states
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