

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



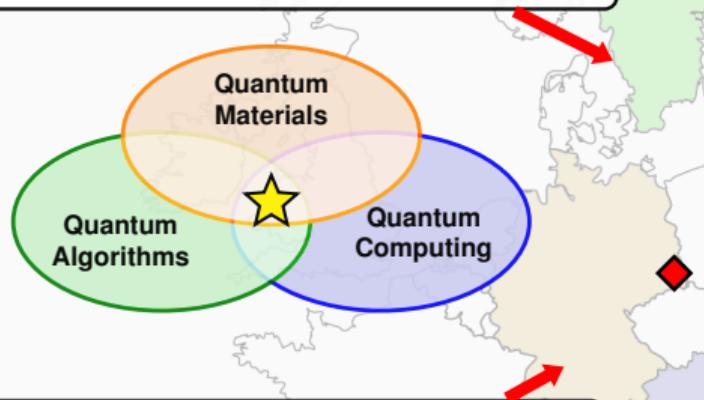
FUNDED BY



My Background

PostDoc – Quantum Computing

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



Academic Network



WACQT Wallenberg Centre for Quantum Technology

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



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



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



MAX PLANCK INSTITUTE
FOR SOLID STATE RESEARCH

PhD in Computational Chemistry

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

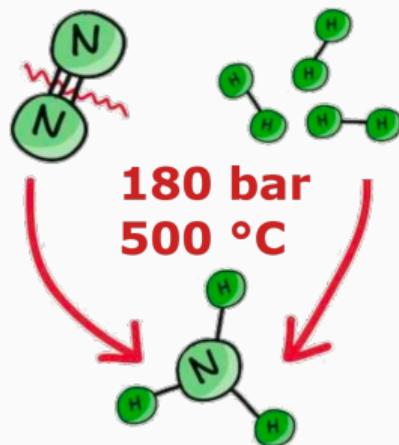


BSc/MSc Studies in Physics

Computational/Solid State Physics

Motivation: Haber-Bosch process and biological nitrogen fixation

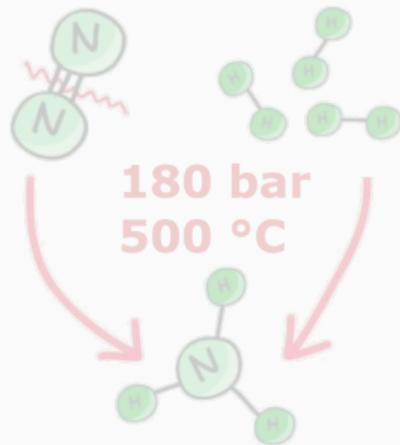
Haber-Bosch Process



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

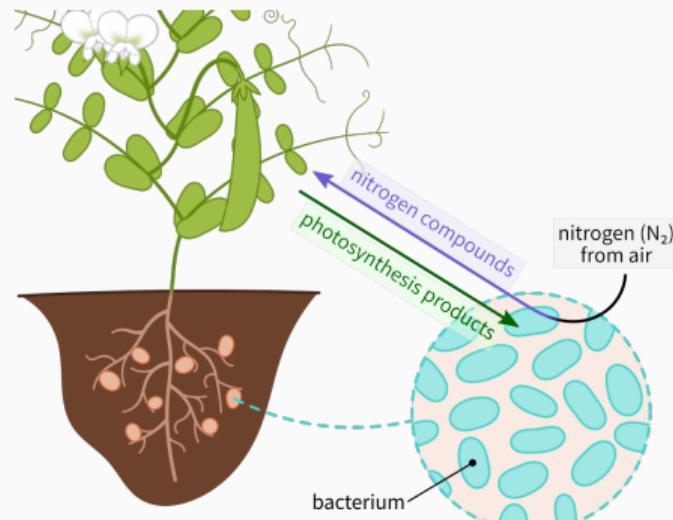
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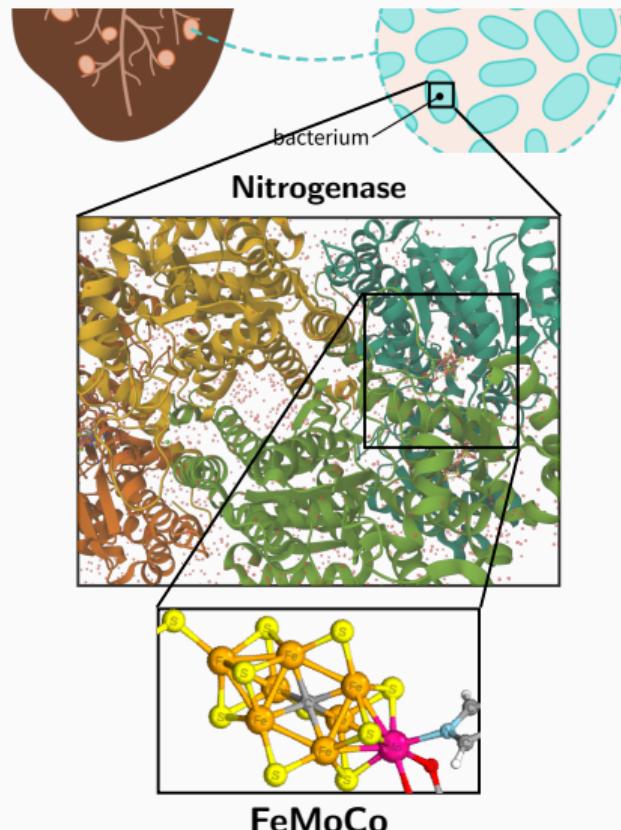
Biological nitrogen fixation



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

Problem: Strongly correlated transition metal compounds

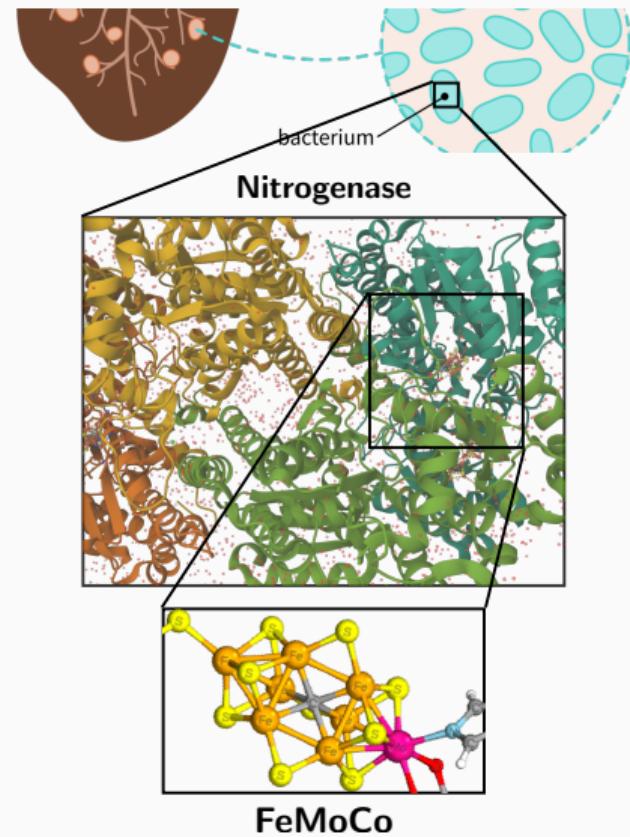
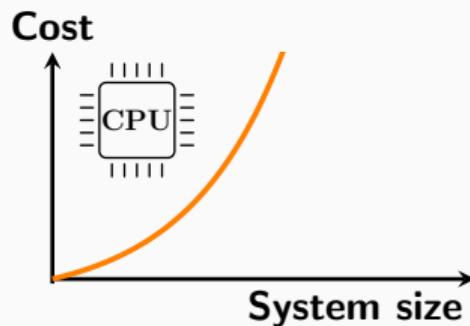
- **Transition metal clusters** act as catalysts:
Iron-Molybdenum cofactor (FeMoCo) and
other iron-sulfur clusters
- **Experimental study very difficult!**



Problem: Strongly correlated transition metal compounds

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

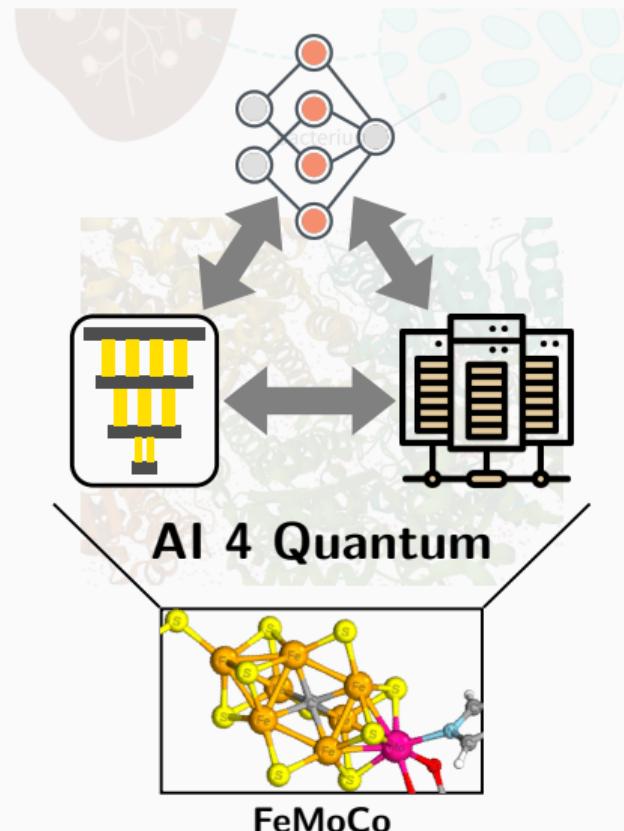
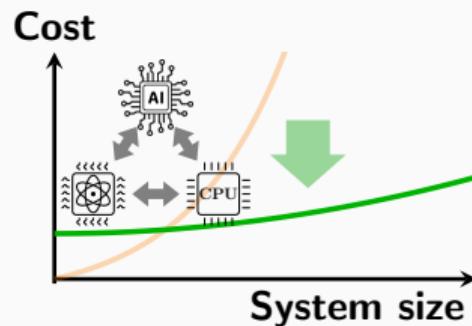
We have the equations at hand, but
exponentially costly on classical computers!



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

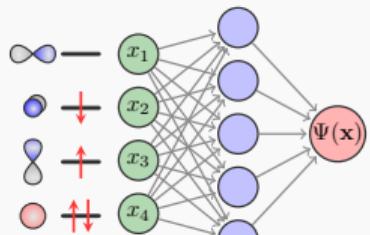


AI 4 Quantum

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

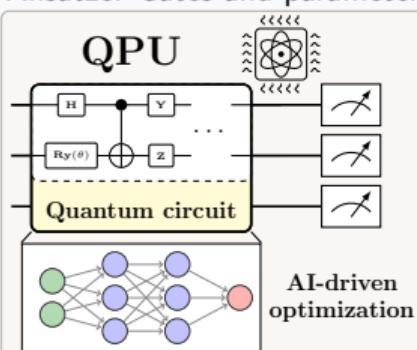
Neural Network States for Quantum Matter

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



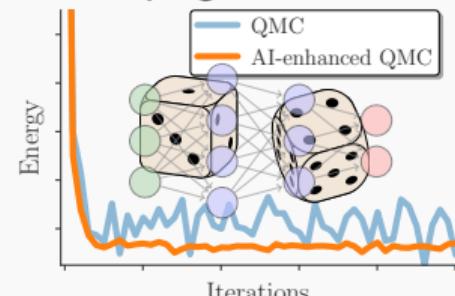
AI-driven Quantum Computing Approaches

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



AI-enhanced Quantum Monte Carlo Methods

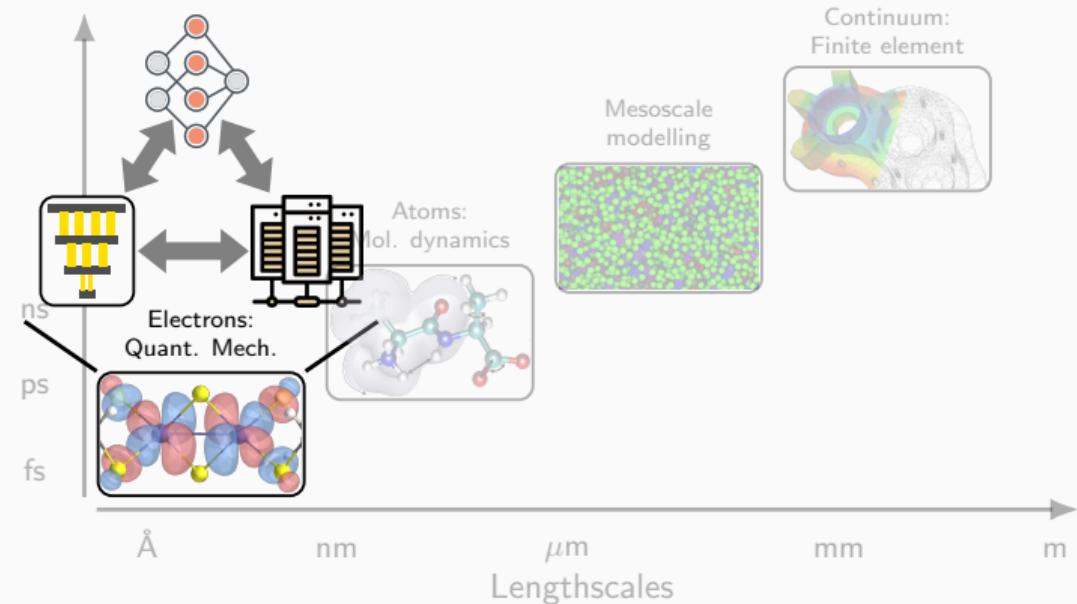
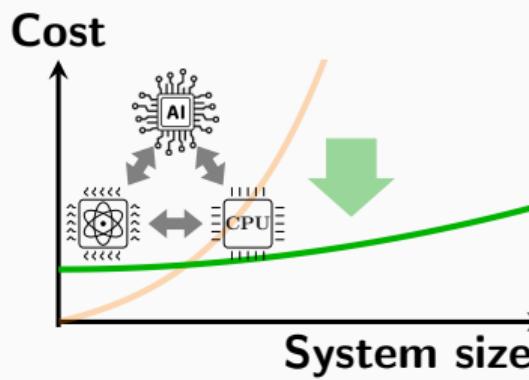
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AI 4 Quantum – Overview

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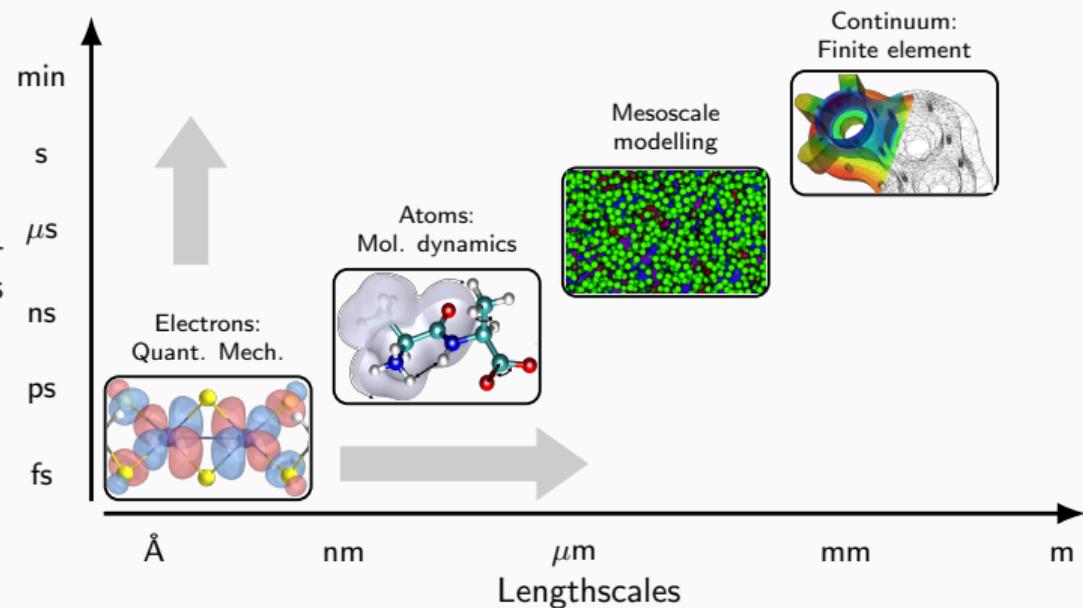
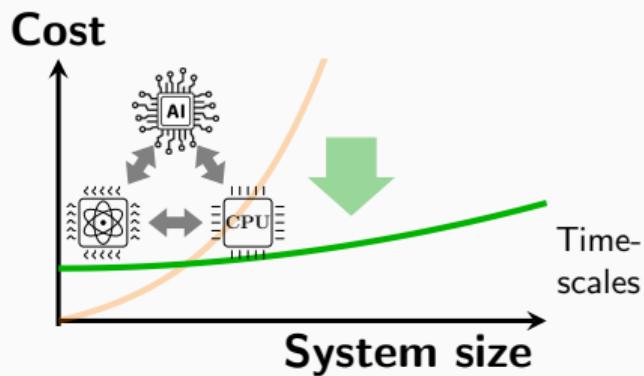
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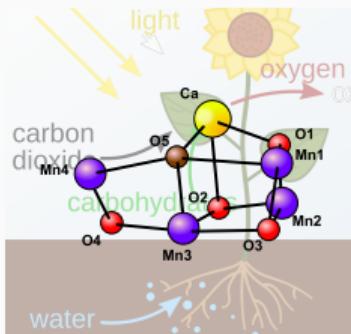
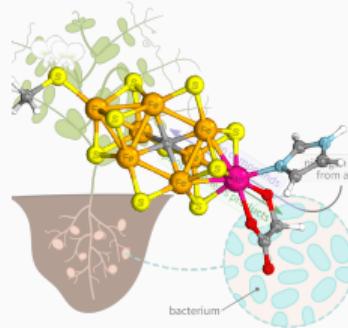
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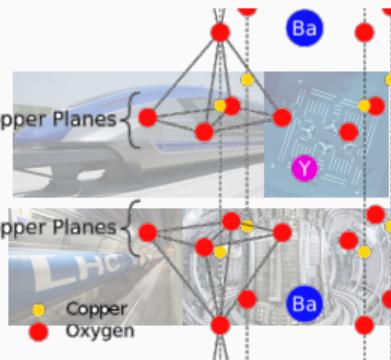
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Nitrogen fixation

Artificial photosynthesis

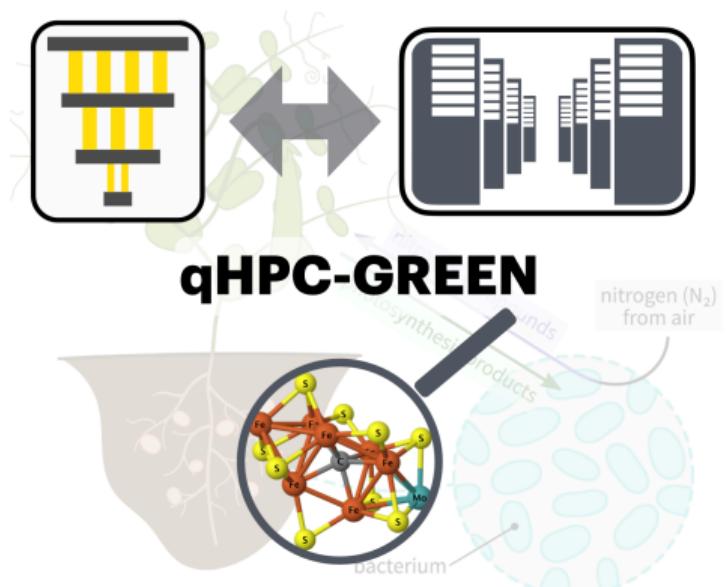


High- T_c superconductivity

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

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

AI 4 Quantum – Funding



1.8M EUR

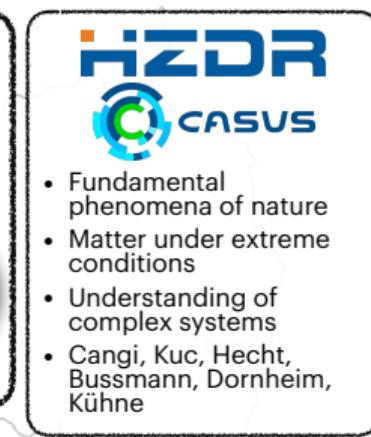
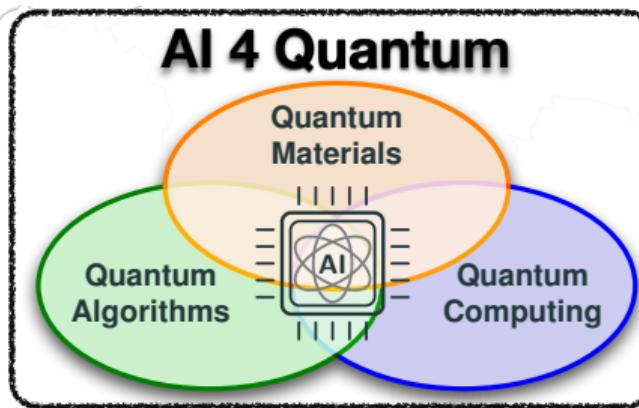
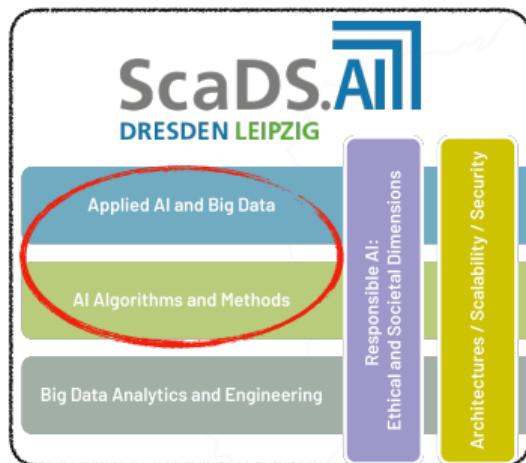
HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES
Helmholtz Investigator Group

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



CHAIR OF
MATERIALS SCIENCE
AND NANOTECHNOLOGY



CHAIR OF THEORETICAL
CHEMISTRY



DRESDEN
concept



Scientific Area Committees:

- Information Technology & Microelectronics
- Materials & Structures



AI 4 Quantum – Hiring and Acknowledgements

Group



PhDs



PostDocs

I AM HIRING!

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

**Funding and
Acknowledgements**



Bundesministerium
für Bildung
und Forschung



SACHSEN
concept

DRESDEN
concept



HELMHOLTZ
HZDR
CASUS

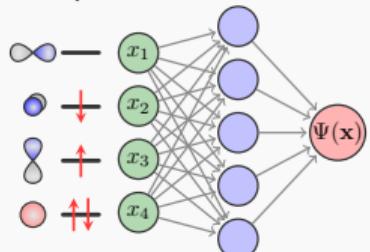
Thank you for your attention!

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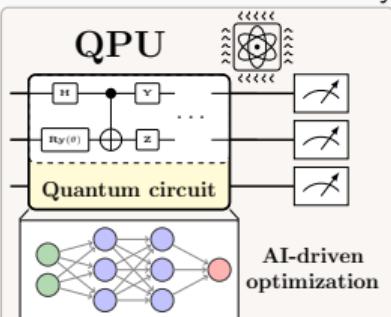
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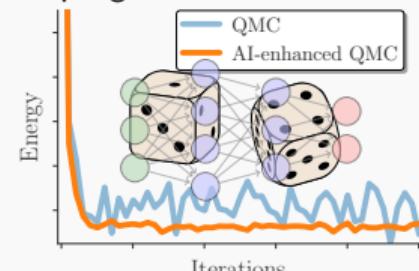
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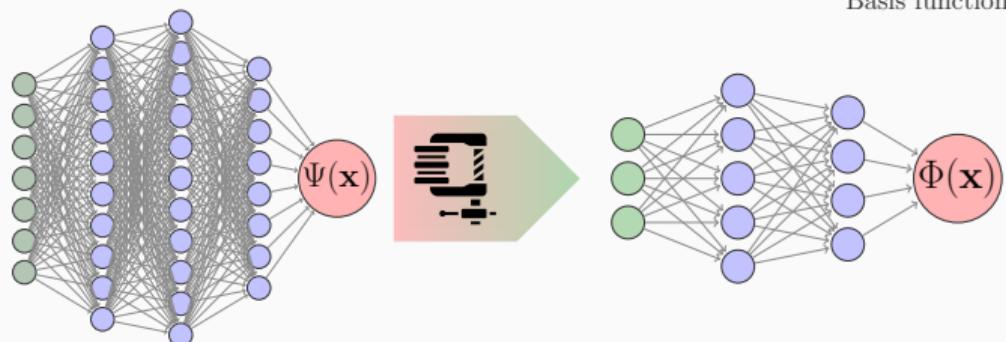
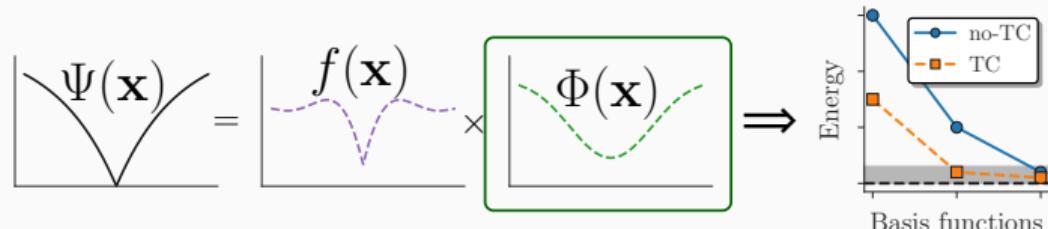
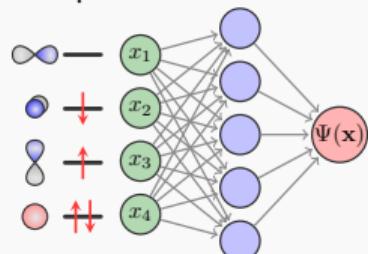


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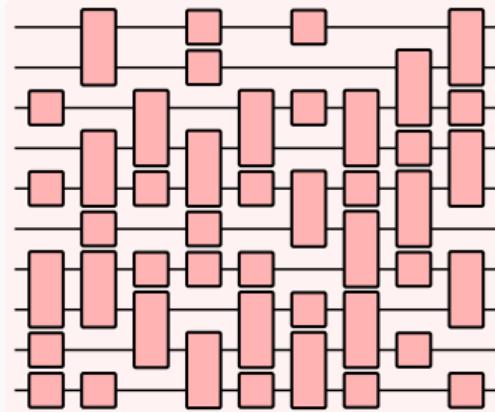
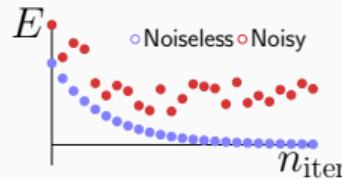
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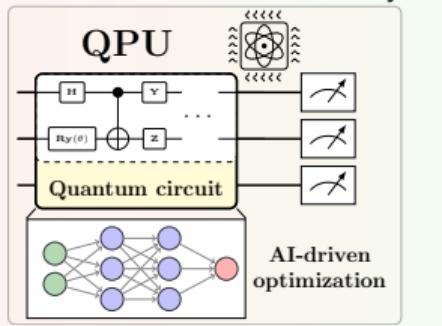


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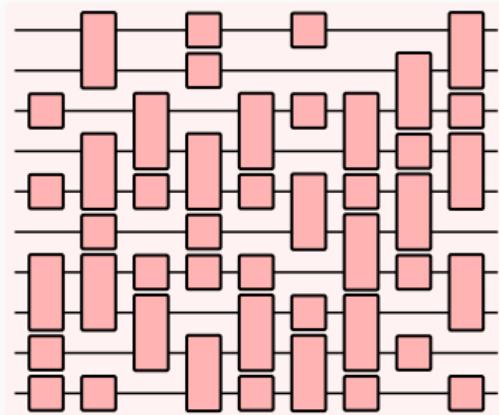
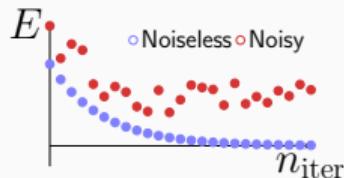
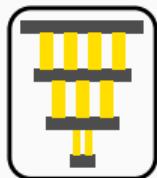


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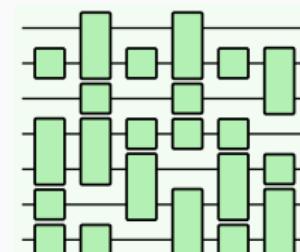
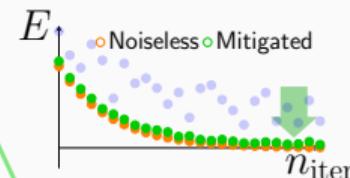
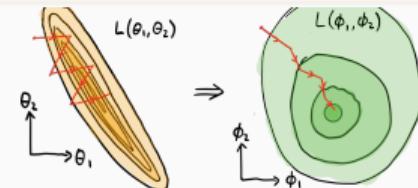
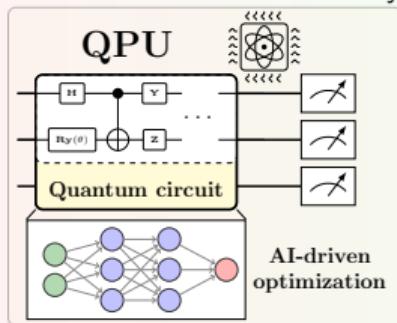
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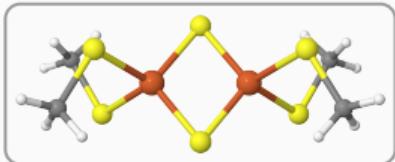
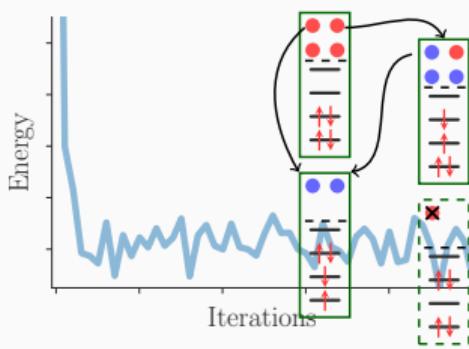
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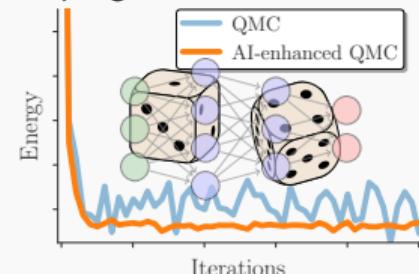
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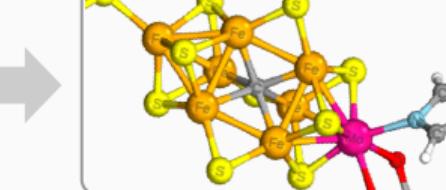
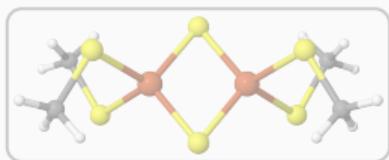
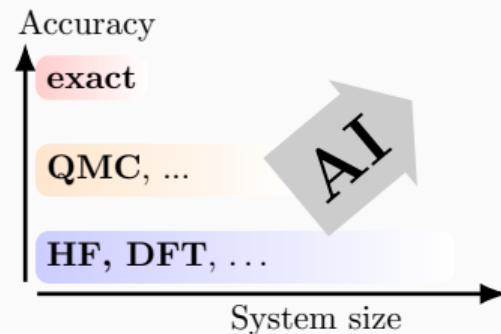
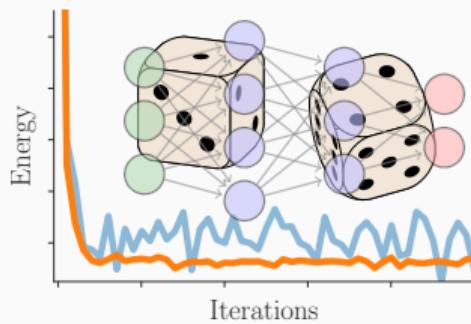
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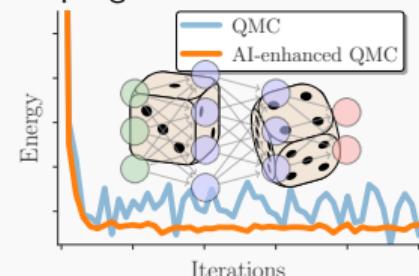
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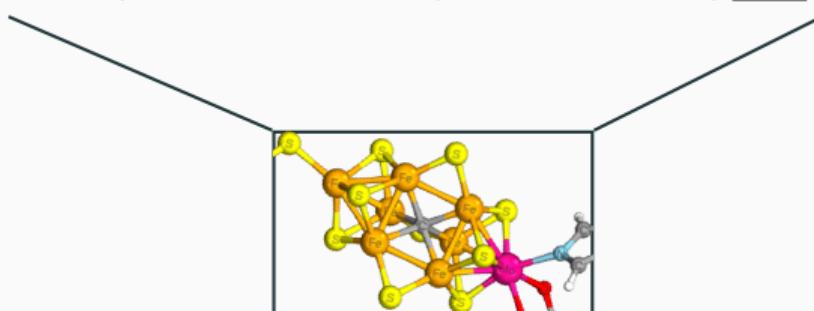
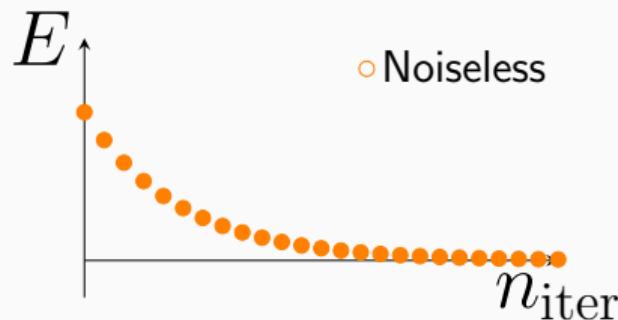
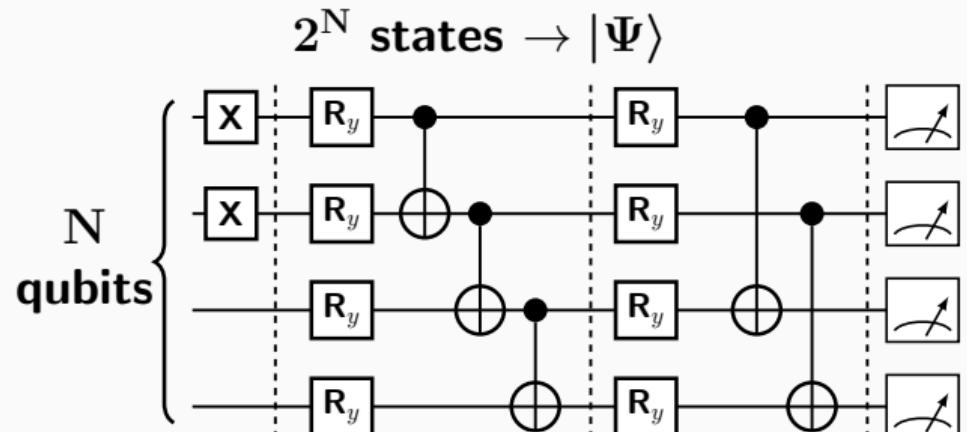
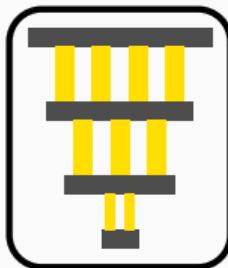


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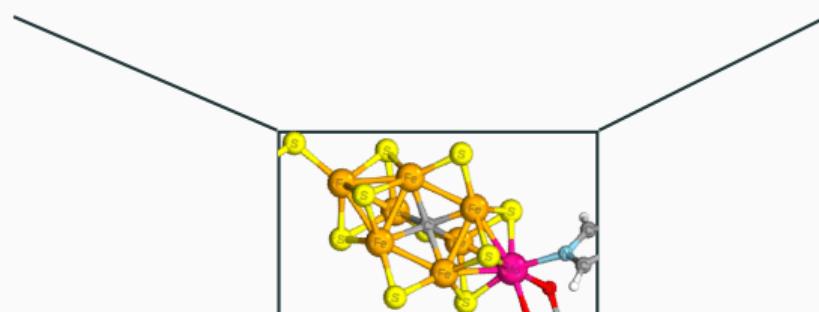
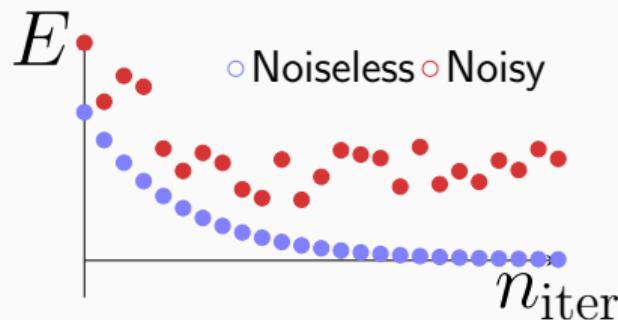
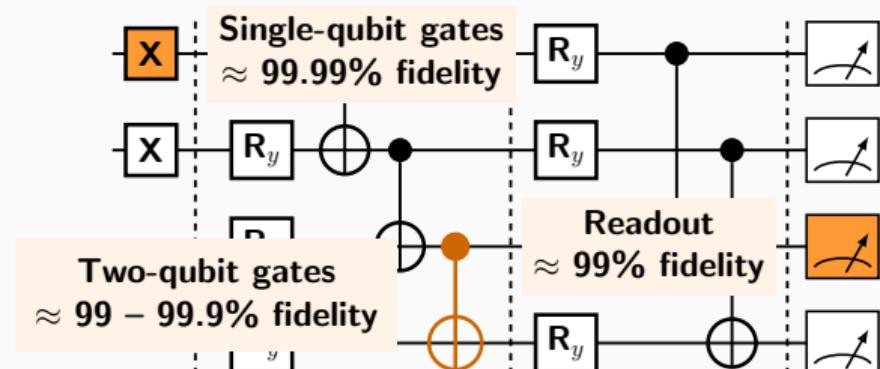
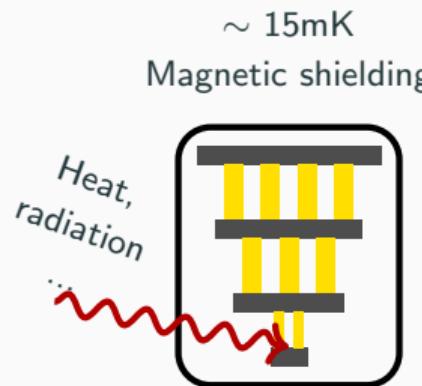
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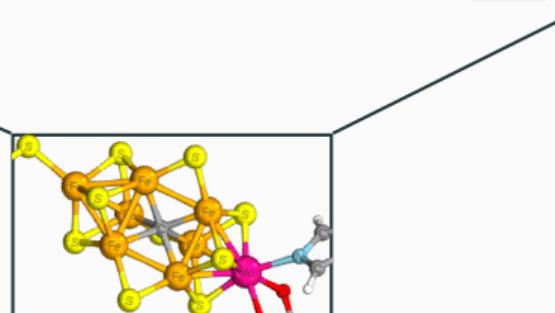
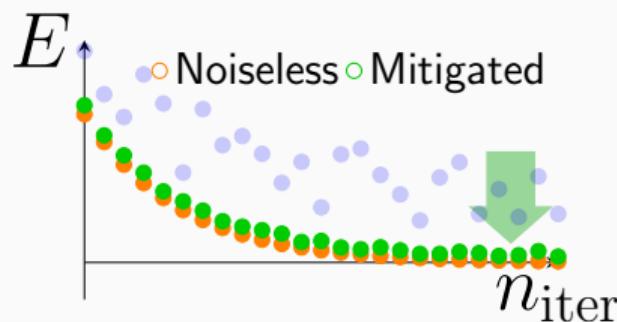
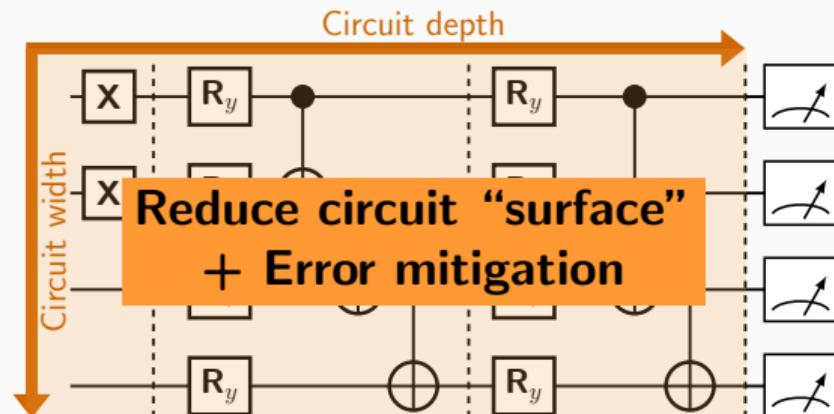
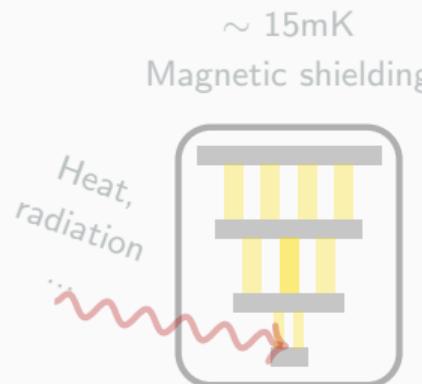
Problem: Noisy intermediate-scale quantum devices



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qHPC-GREEN – Overview

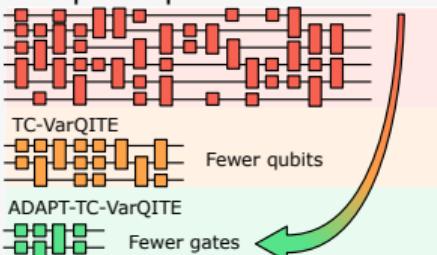
HPC+QC toolkit to study strongly correlated quantum chemistry problems

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

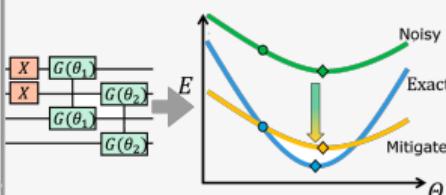
WP1

Resource reduction:

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

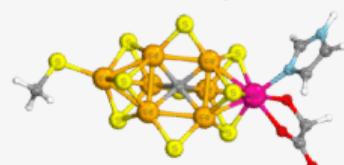


Error mitigation:



Relevant applications:

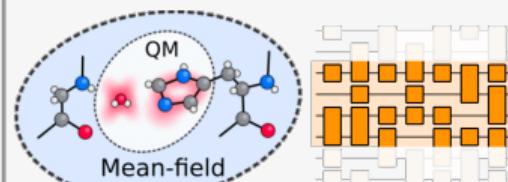
Electronic structure of transition metal complexes



WP2

Algorithms and software for relevant insights:

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



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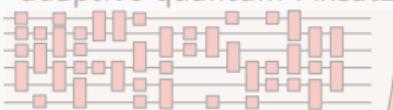
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TC-VarQITE

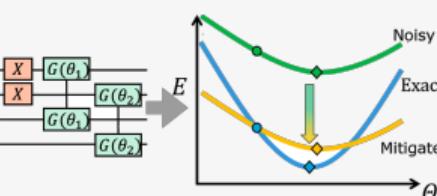
Fewer qubits

ADAPT-TC-VarQITE

Fewer gates

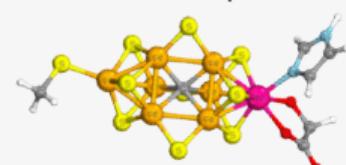
WP1-2

Error mitigation:



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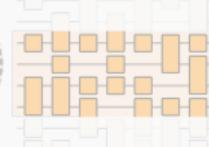
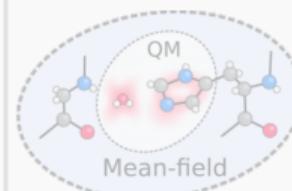
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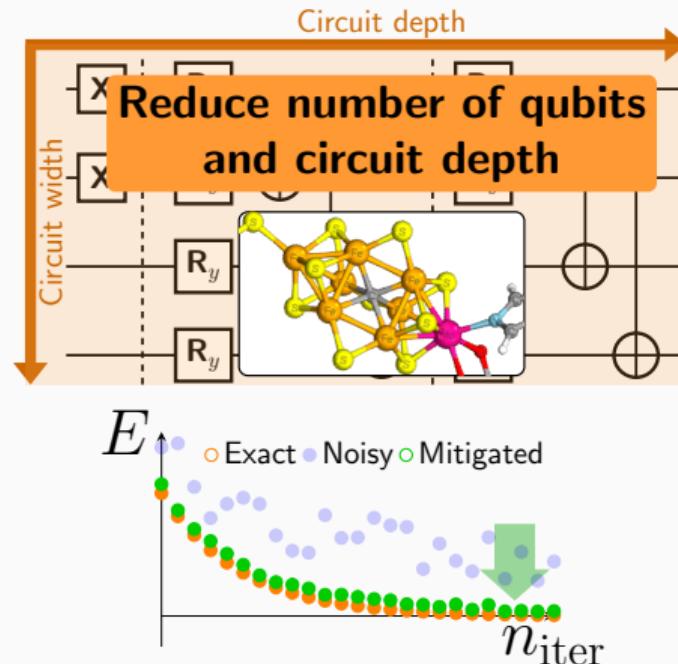
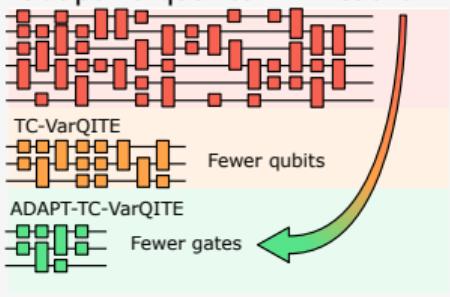
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Resource Reduction

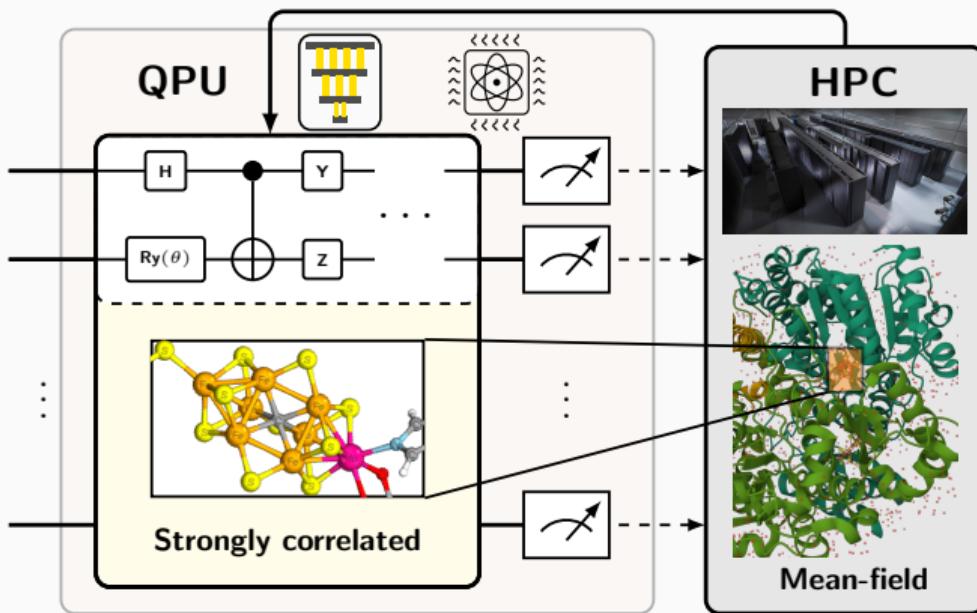
- Accurate calculations for relevant problems on current and future NISQ devices
- Transcorrelation, active spaces, spin-symmetry and adaptive quantum Ansätze



qHPC-GREEN – Overview

HPC+QC toolkit to study strongly correlated quantum chemistry problems

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



WP2

Algorithms and software
for relevant insights:

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

