

## Machine learning for quantum simulation and quantum computing

Group Leader at CASUS/HZDR and ScaDS.AI/TUD

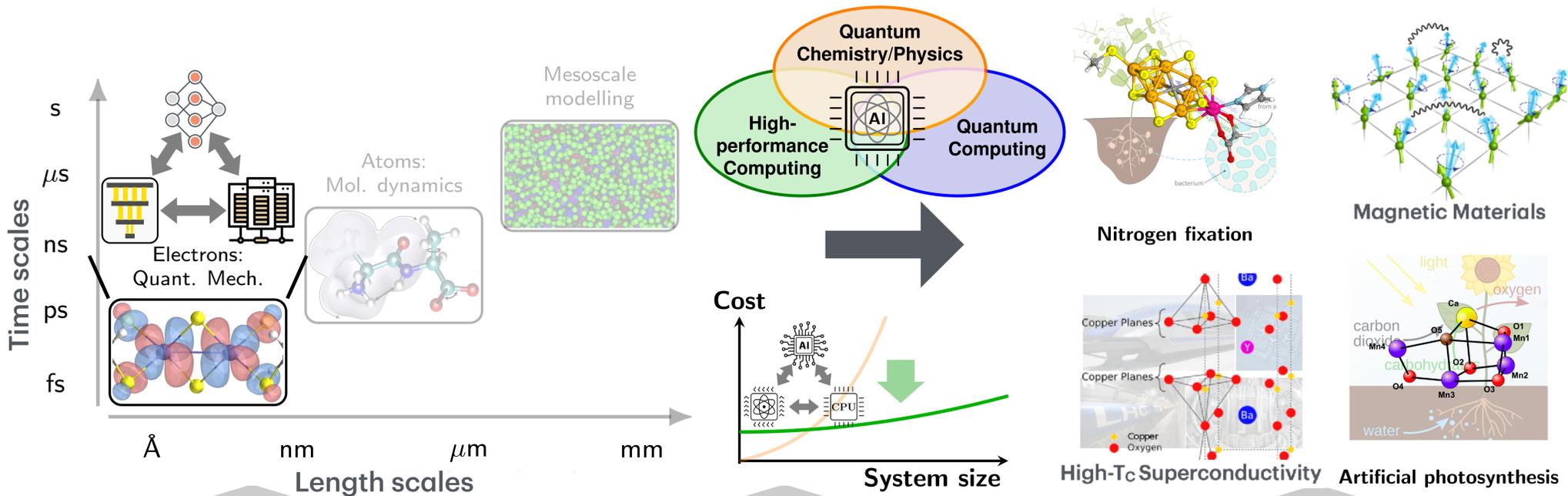
[w.dobrautz@hzdr.de](mailto:w.dobrautz@hzdr.de)

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### 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

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

## HPC+QC algorithms toolkit to study strongly correlated electron problems

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

### WP1

#### Resource Reduction

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

TC-VarQITE: Fewer qubits

ADAPT-TC-VarQITE: Fewer gates

### WP2

#### Quantum Error Mitigation

#### Relevant Applications:

Electronic structure of transition metal compounds

#### Algorithms and Software for relevant insights:

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