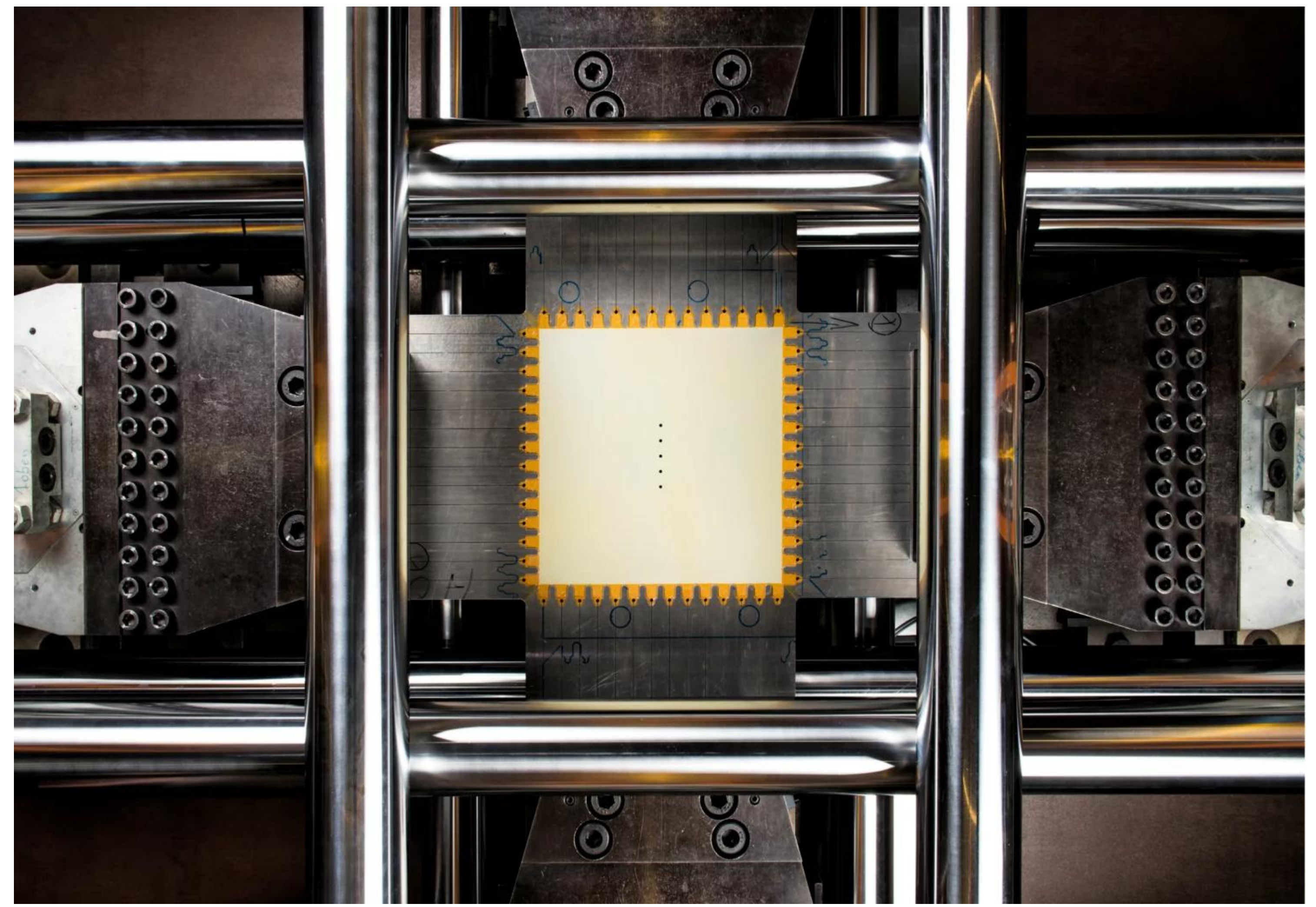


# QuantiCoM

## Quantum Computing for Materials Science and Engineering

We are exploring tools for the rapid discovery and development of new materials, their transfer to industrial partners for application, and the identification of simulation approaches that promise quantum advantage.

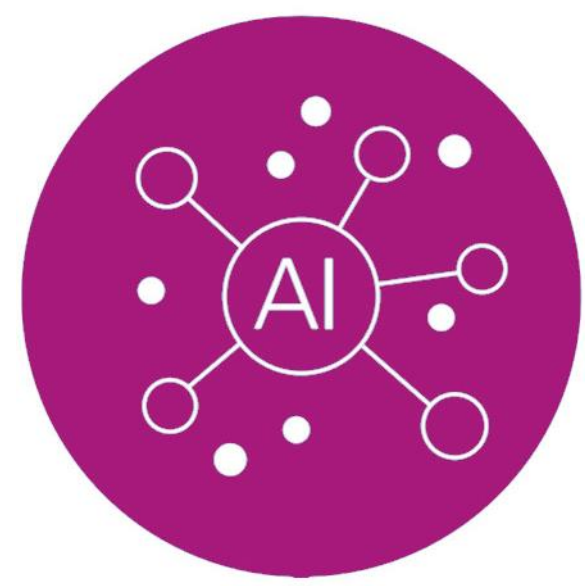
- Applications
- Materials science



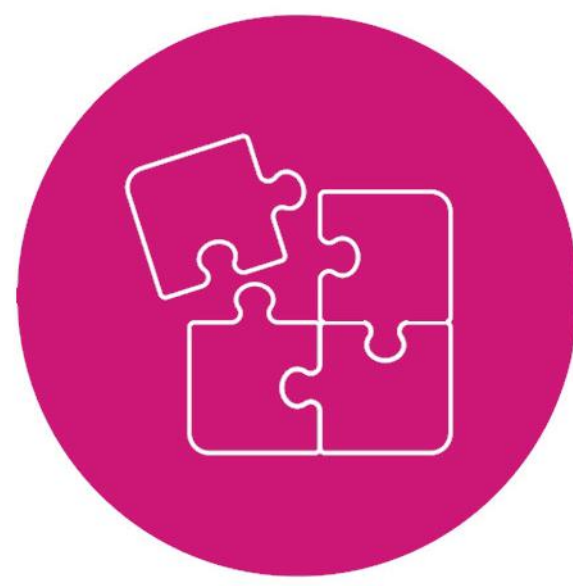
### Development of QC and Hybrid Algorithms

### QC/HPC Atomistic Simulations and QML

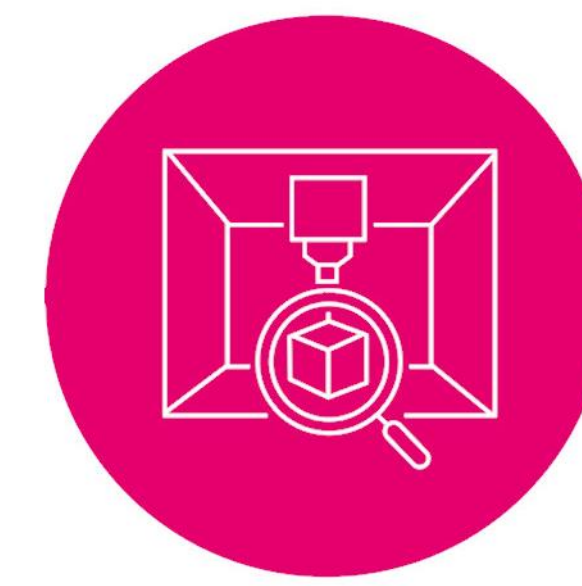
### New Materials and Rapid Validation



Machine learning for rapid analysis



Materials combinatorics



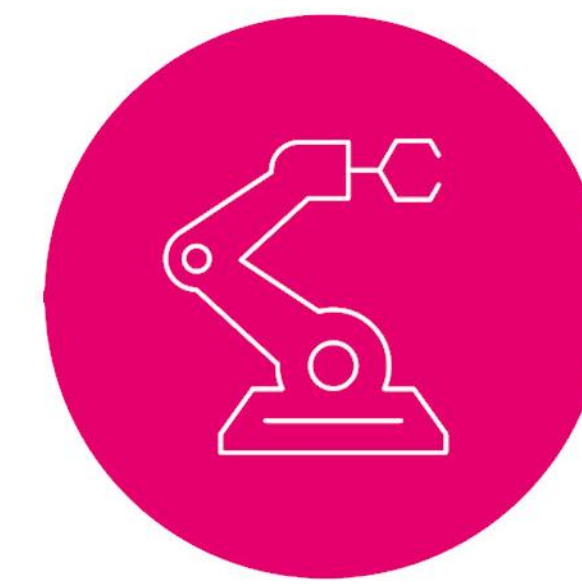
In situ and operando experiments



Predictive simulations



Multiscale simulations



Self-driving labs

### Bridge QC-Materials

### Use Cases

### Validation and Transfer

- Quantum simulation of model systems
- Development of hybrid algorithms for atomistic simulations
- Quantum machine learning

- Interaction H/O/H<sub>2</sub>O with metals
- Stability of strongly correlated materials
- Combination of QC simulations and machine learning

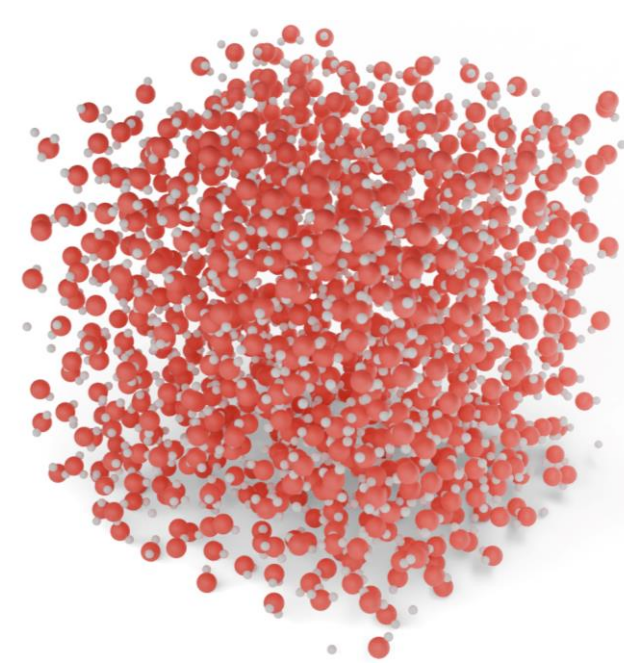
- Digital services for case studies in materials science
- High-throughput generation of experimental data
- High-throughput CALPAHD-based materials design

## Industry

### Development of Algorithms for Atomistic Simulations

### Use Cases Materials Science and Materials Engineering

- Dynamics of H<sub>2</sub>O  
Classical and QC-modeling of water on HPC and QC hardware
- Quantum machine learning  
QML for materials optimization and screening to predict and optimize material properties
- Quantum embedding theories  
Implementation of QC for active regions in conventional simulations to handle strongly correlated systems



- Materials Degradation  
Atomic interactions between H/O/H<sub>2</sub>O with intermetallic compounds → Corrosion of Al-alloys
- Thermodynamics  
Stability of compounds with strong and weak electronic correlations embedded in metallic environments
- Accelerated materials development  
Complex optimization tasks for high-throughput CALPHAD-based materials development

Mehr Infos zu dem Projekt auf unserer Website.



Ein Projekt von



Auftragnehmer



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Get in touch.  
We enable quantum!



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