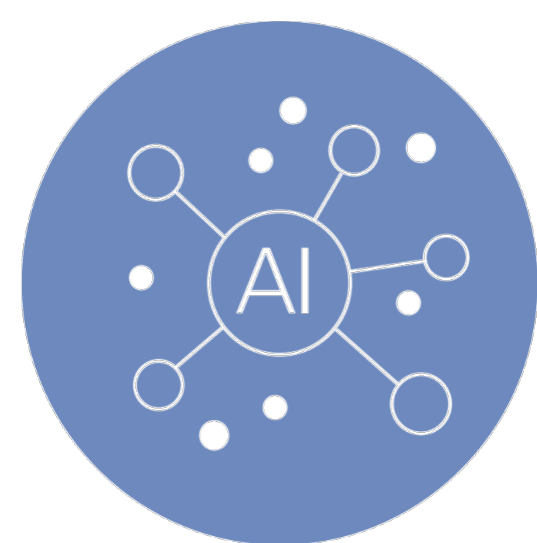


QuantiCoM

Quantum Computing for Materials Science and Engineering

Development of QC and Hybrid algorithms

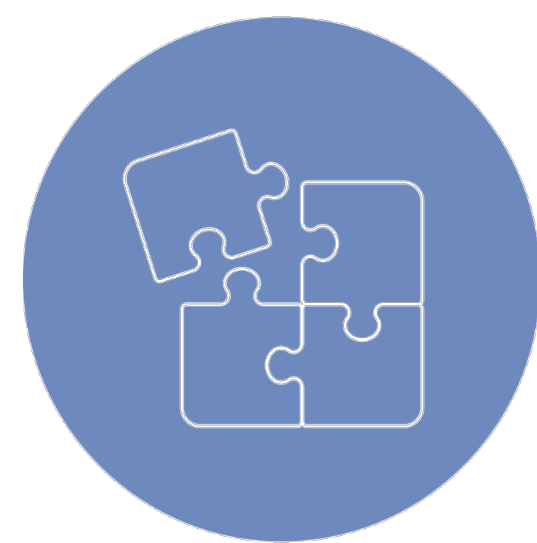


Machine learning for rapid analysis



Predictive simulations

QC/HPC atomistic simulations and QML

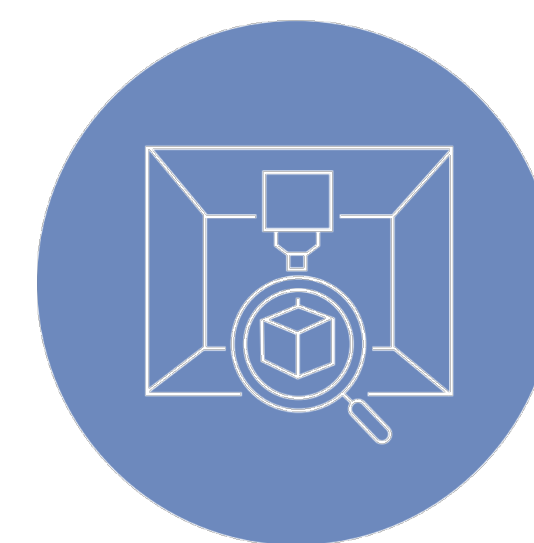


Materials combinatorics

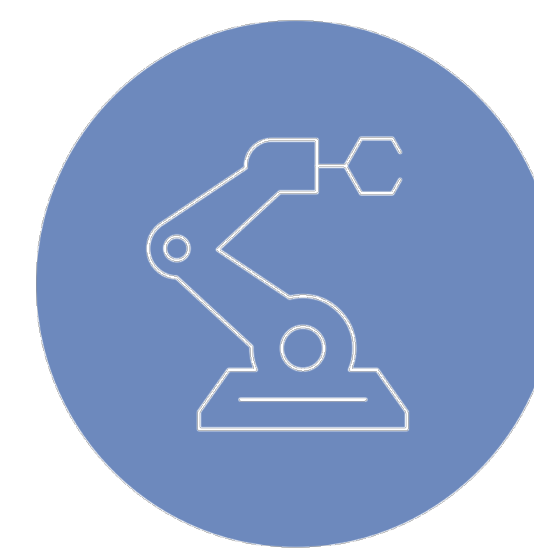


Multiscale simulations

New materials and rapid validation



In situ and operando experiments



self-driving labs

Bridge QC-Materials

- Quantum simulation of model system
- Development of algorithms for atomistic simulations
- Quantum Machine Learning

Use Cases

- Interaction H/O/H₂O with metals
- Stability of strongly correlated systems
- Combination of QC simulations and machine learning

Validation and Transfer

- Digital services for case studies
- High-throughput experimental data generation
- High-throughput CALPAHD-based design

Industry

Development of algorithms for atomistic simulations

- Molecular Dynamics of H₂O
 - Classical and qc-modeling of water on HPC and QC hardware and benchmarking
- Quantum machine learning
 - QML for materials optimization and screening to find global minima.
- Quantum embedding theories
 - Implementing active spaces in classic atomistic simulations to handle strongly correlated systems

Use Cases Materials Science and Materials Engineering

- Materials Degradation
 - Atomic interactions between H and O as single elements and in the form of H₂O with metallic elements.
- Thermodynamics
 - Stability of compounds with strong and weak electronic correlations embedded in metallic environments
- Accelerated materials development
 - Optimization tasks for high-throughput CALPHAD-based materials development

We are hiring!

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