# QCMineral
Quantum-Classical Material Development Platform for Industrial Applications

We develop quantum computing-based atomistic simulation approaches for the investigation of compositional and doping effects in structurally complex crystalline and amorphous oxide materials with the aim of optimizing process-relevant material characteristics for industrial applications.
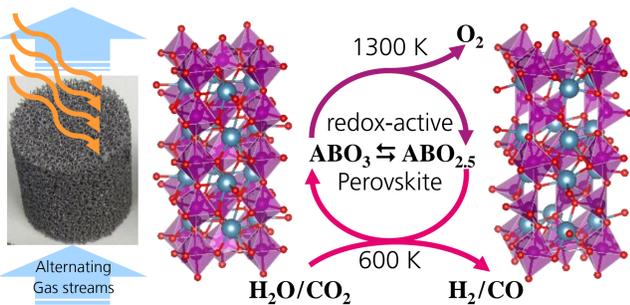
- Applications
- Materials Science
- Energy
- Sustainability
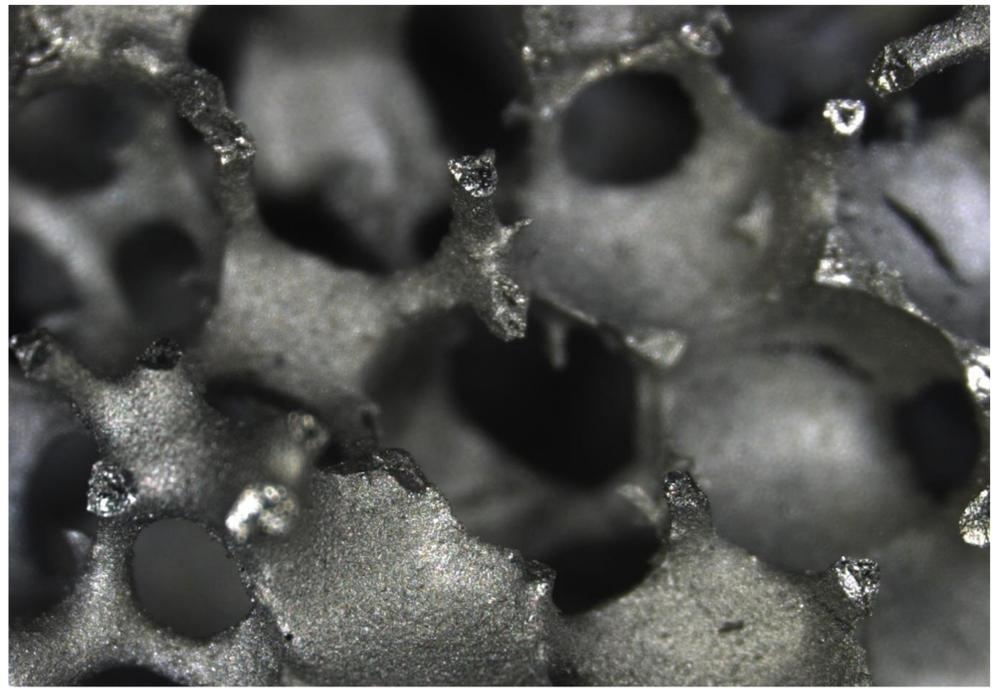
Project Challenges

Accurate description of *highly correlated electrons* in functional oxide materials

⇒ *Redox materials*, *glasses* and *glass ceramics*

Prohibitive *exponential scaling* with system size of wave-function based quantum chemistry approaches on classical HPC hardware

⇒ Implementation of *QC algorithms* for periodic systems with favorable scaling

Redox Materials for Solar-Thermal Water Splitting

New technology for solar fuels

1300 K → O_2

redox-active
$ABO_3 \leftrightharpoons ABO_{2.5}$
Perovskite

600 K

Alternating Gas streams

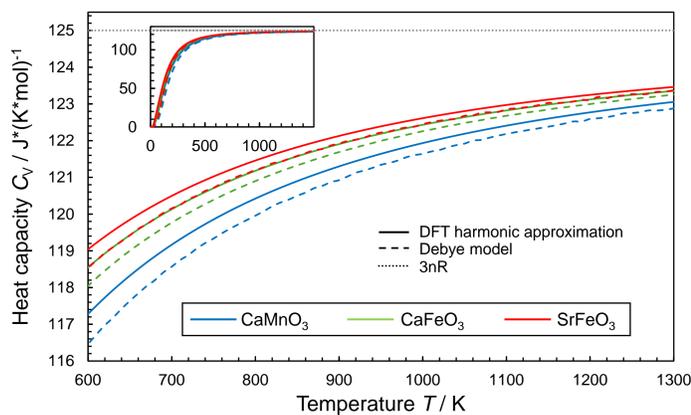H_2O/CO_2 → H_2/CO

Heat Capacity $C_V(T)$

DFT Harmonic Approach

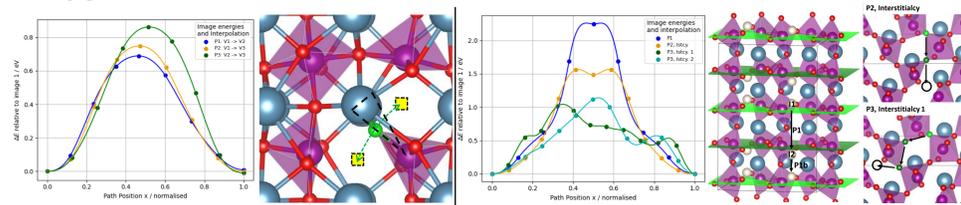$$C_V = \sum_{i=0}^{3N} \frac{(h\nu_i)^2}{k_B T^2} \frac{e^{(h\nu_i/k_B)}}{\left(e^{(h\nu_i/k_B)}-1\right)^2}$$

Debye model

$$C_V = 9R\left(\frac{T}{\Theta_D}\right)^3 \int_0^{T/\Theta_D} \frac{x^4 e^x}{(e^x-1)^2} dx$$

Debye Temp.: $\Theta_D = \frac{h\nu}{k_B}\left(\frac{6N}{\pi V}\right)^{1/3}$

- DFT harmonic approximation
- Debye model
- 3nR

CaMnO₃ CaFeO₃ SrFeO₃

Oxygen diffusion mechanism at δ≈0 and in ordered vacancy structure at δ≈0.5

## Amorphous Glasses and Glass Ceramics

Structure generation

○ Classical and ab initio molecular dynamics (MD) simulations for the complex atomic structure of proto-typical glass-forming SiO_2 - oxides and glass ceramics.
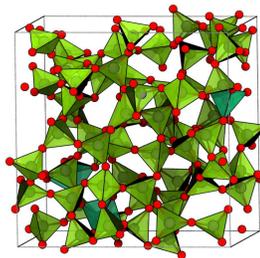

SiO_4 coordination polyhedra representation of a DFT-relaxed 216 atom unit cell amorphous silicon dioxide (a-SiO₂).

○ Prediction of macroscopic material properties based on their microscopic structure; validation against electron and neutron diffraction data.
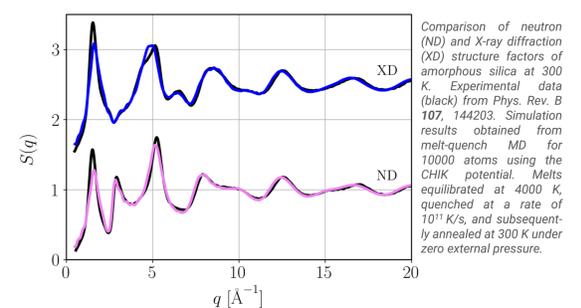

Comparison of neutron (ND) and X-ray diffraction (XD) structure factors of amorphous silica at 300 K. Experimental data (black) from Phys. Rev. B 107, 144203. Simulation results obtained from melt-quench MD for 10000 atoms using the CHIK potential. Melts equilibrated at 4000 K, quenched at a rate of 10^{11} K/s, and subsequently annealed at 300 K under zero external pressure.
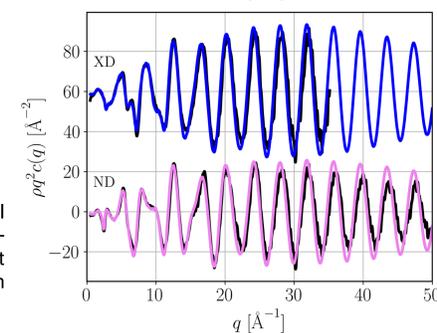
Direct correlation function c(q) of amorphous silica at 300 K, obtained from the neutron and X-ray diffraction structure factors above scaled by the factor ρq^2.

Quantum Mode-Coupling Theory (QMCT)

○ Prediction of the relevance of quantum effects for dynamical properties of liquids in an supercooled regime by extension of classical mode-coupling theory (MCT).

○ Application of QMCT to specific model systems of glass forming materials; Benchmarking against state-of-the-art ab initio theory for complex systems.

○ Path integral simulations and testing of feasibility on quantum hardware.
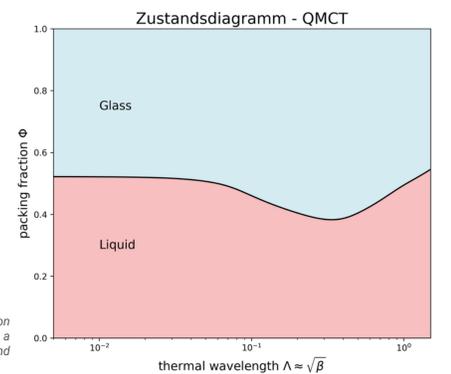
State diagram of the QMCT: Transition between liquid and glass phase as a function of thermal wavelength and packing density.
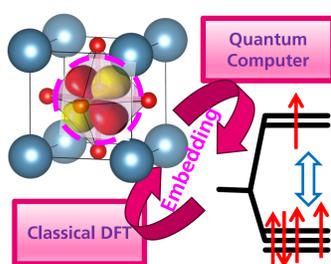
Industry Projects

QUADRANT
QUantum ADvantages for Redoxmaterial Application through Novel Technologies

<u>HPC-QC hybrid algorithms</u>
Embedding of QC active site into conventional HPC simulations for strongly correlated electrons

<u>Accurate Energetics</u>
Improved modeling of thermodynamical and transport properties of redox materials
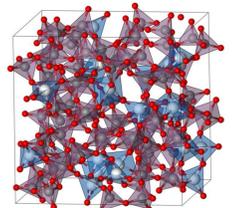

QUADRIGA
QUAntum Dynamics Research for Innovative Glass Applications
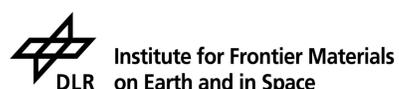
<u>Modifications & Compositions</u>
QC / HPC modeling of crystalline/amorphous states

<u>Dynamic properties</u>
Glassy dynamics and crystallization in glass ceramics

<u>Accelerated materials development</u>
Machine-learning supported development of novel functional oxides

Ein Projekt von

DLR — Institute for Frontier Materials on Earth and in Space

DLR — Institute of Future Fuels

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DLR | QCi

Get in touch.
We enable quantum!

Mehr Infos zu dem Projekt auf unserer Website https://qci.dlr.de/qcmineral/