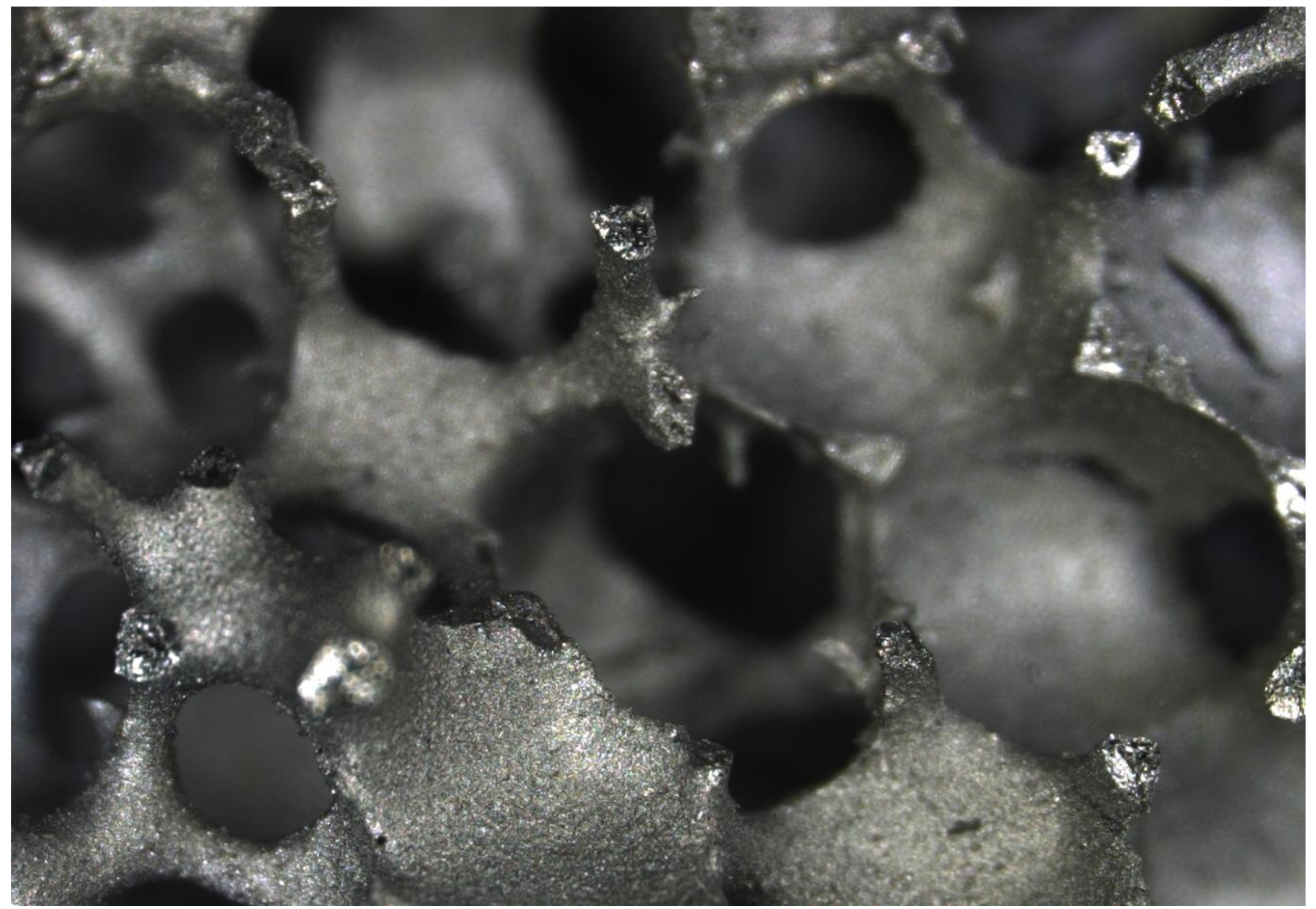


# QCMineral

## 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



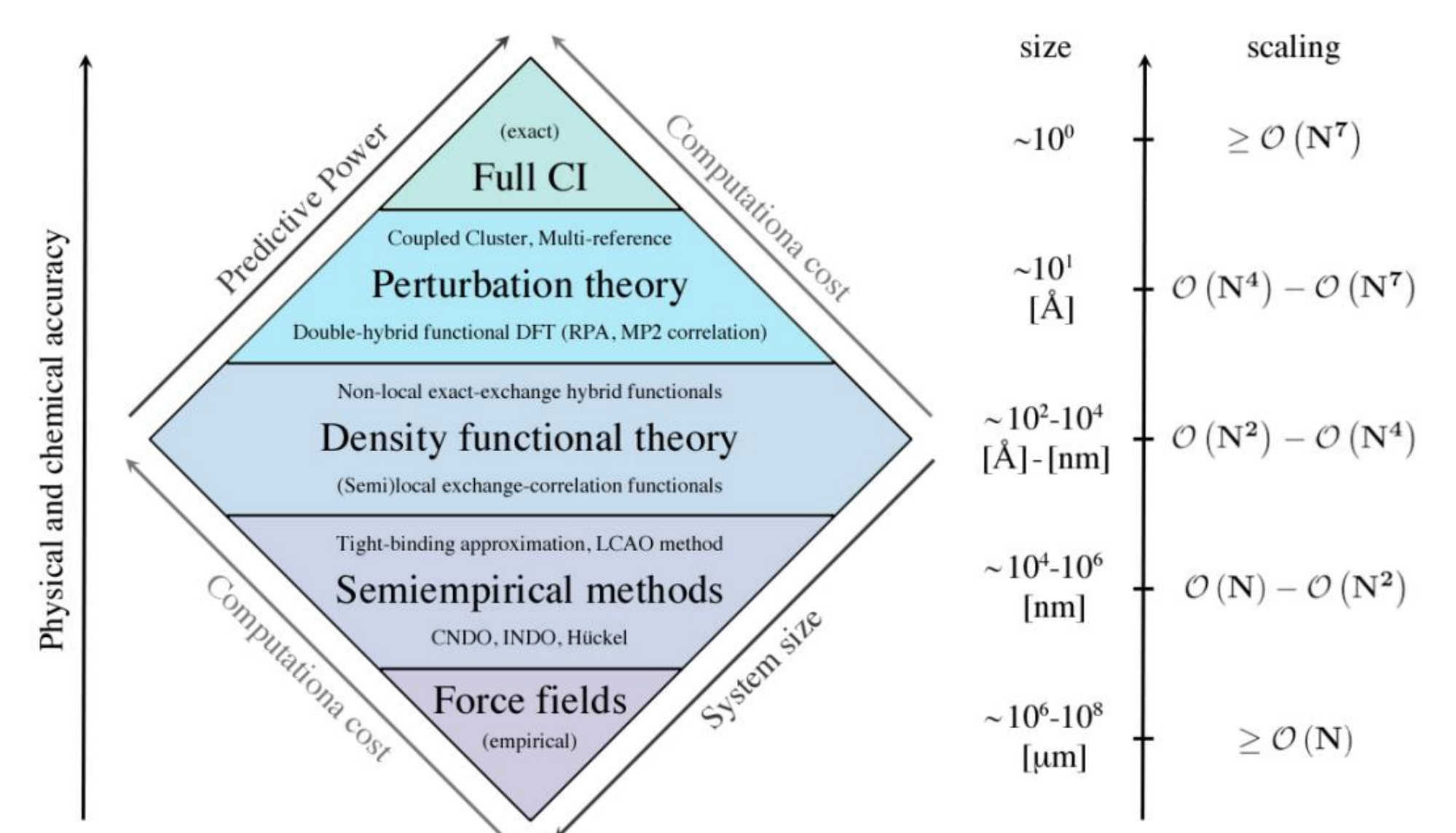
### Project Challenges

Accurate description of highly correlated electrons in functional oxide materials  $\Rightarrow$  *redox materials*, *glasses* and *glass ceramics*

Prohibitive *exponential scaling* with system size of conventional quantum chemistry approaches on classical HPC hardware

$\Rightarrow$  Implementation of *QC algorithms* for periodic systems with favorable scaling

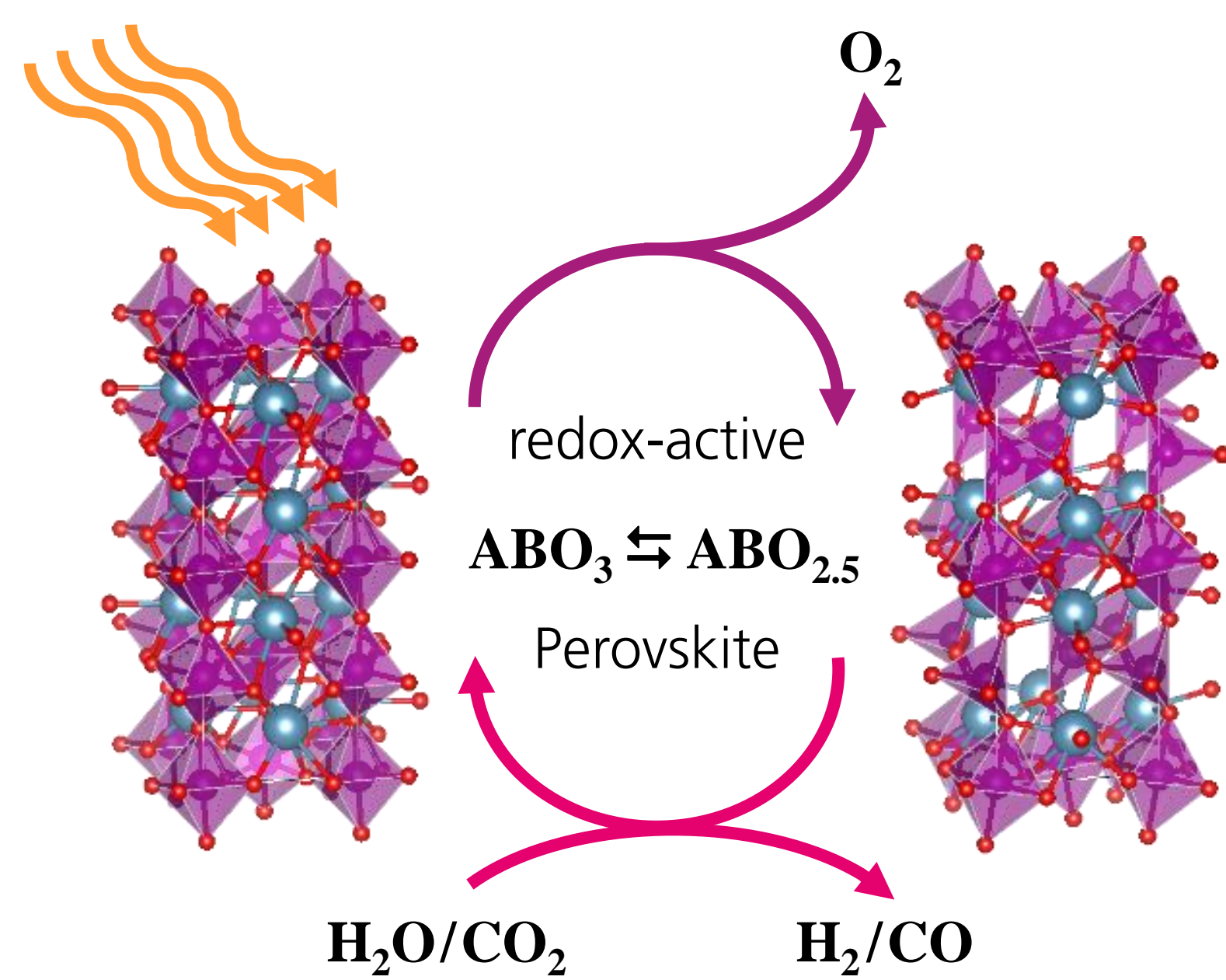
Thorough screening of complex *chemical composition* spaces of technologically relevant oxide alloys



### Redox Materials for Solar-Thermal Water Splitting



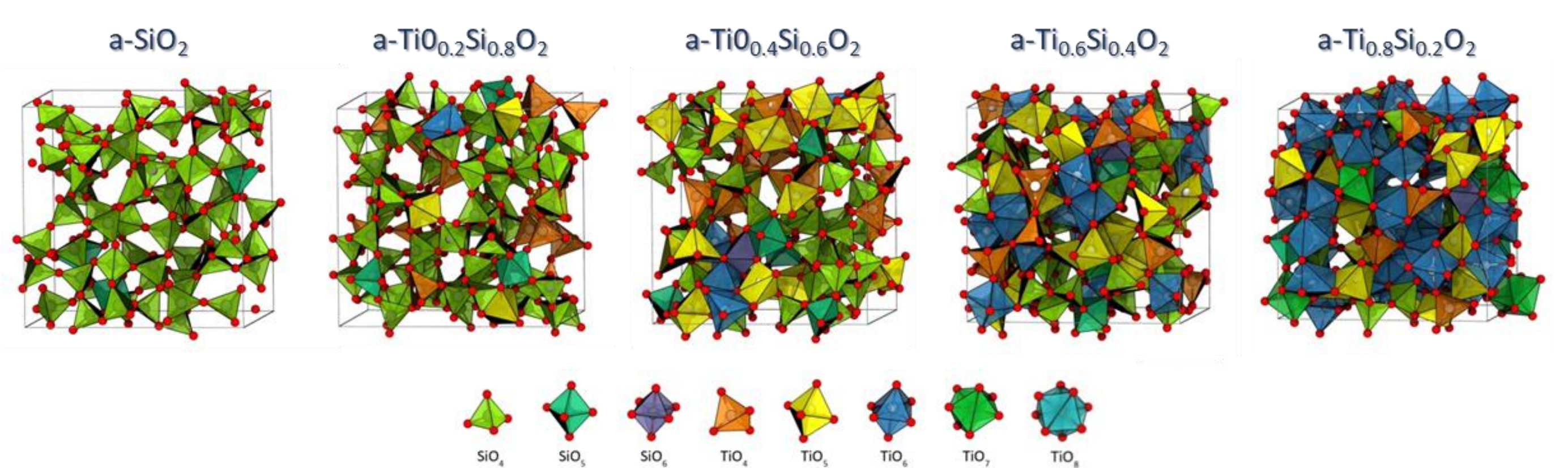
New technology for solar fuels developed at the solar towers in Jülich.



Two-step solar-thermochemical redox-reaction cycle for sustainable fuel production

### Amorphous Glasses and Glass Ceramics

The lack of long-range order/crystalline symmetry in amorphous solids necessitates large unit cells



Microscopic view on composition dependence of static and dynamic properties of silica glasses

### Industry Projects

#### QUADRANT

Quantum Advantages for Redoxmaterial Application through Novel Technologies

##### Thermodynamics & Dynamics

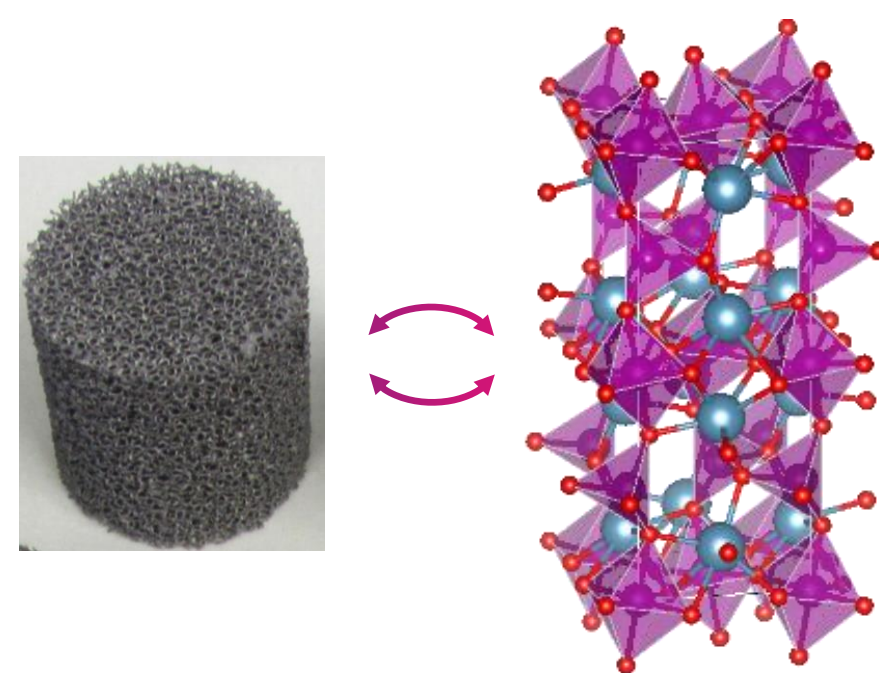
Classical HPC modeling of transport properties of redox materials

##### HPC-QC hybrid algorithms

Embedding of QC into conventional HPC simulations; Strongly correlated oxides

##### Accelerated materials optimization

Materials database for thermodynamic properties and dynamical processes in redox materials



#### QUADRIGA

Quantum Dynamics Research for Innovative Glass Applications

##### Modifications & Compositions

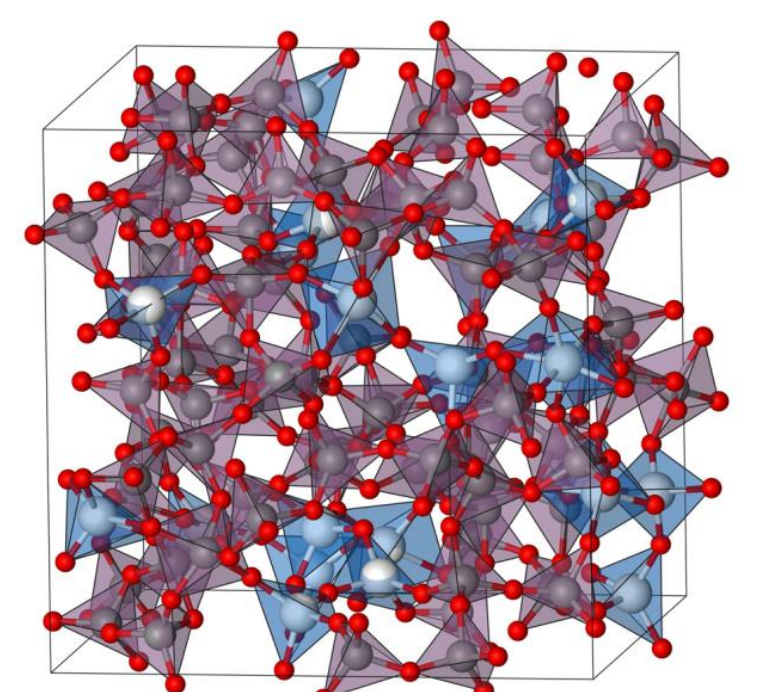
QC/HPC modeling of crystalline and amorphous states as well as crystalline/amorphous mixtures

##### Dynamic properties

Control of glassy dynamics in amorphous solids and crystallization in glass ceramics

##### Accelerated materials development

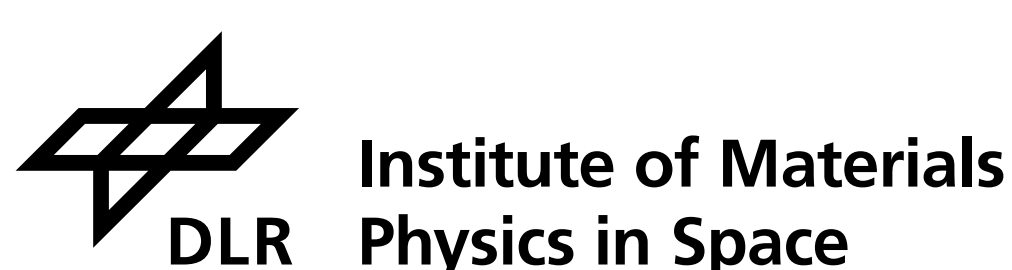
Machine-learning supported development of novel functional oxides



Mehr Infos zu dem Projekt auf unserer Website.



Ein Projekt von

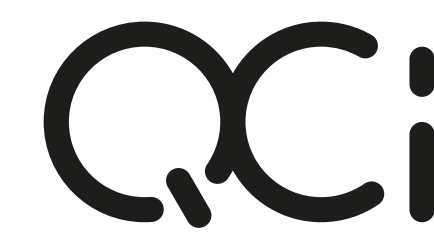


Kontakt

Matthias Sperl  
Matthias.Sperl@dlr.de

Marc Landmann  
marc.landmann@dlr.de

Ulrich Biedermann  
ulrich.biedermann@dlr.de



Get in touch.  
We enable quantum!



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