Quantum Chemistry for Mineral Materials Discovery

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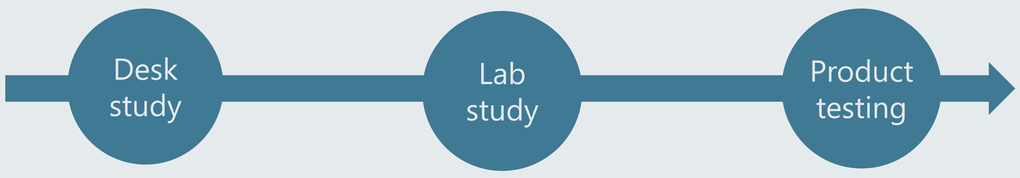
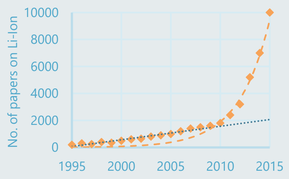
DLR Quantencomputing Initiative

ExoMatter

Problem: Finding new materials is tedious



Example: Finding a new lithium-ion battery cathode material



Too much data

Too many materials to test

System failures

Solution: Material Simulation

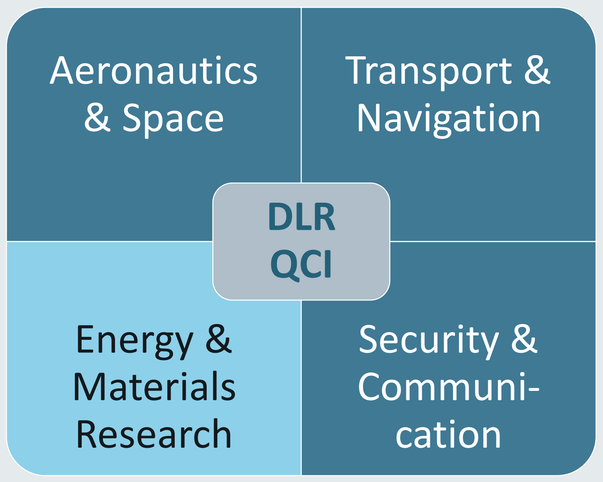
Materials are simulated from first principles through methods such as **Density Functional Theory (DFT)**

1. Simulate the **position and size** of the atoms in a crystal or molecule
2. Simulate the **electrons** around it
3. Move the atoms around and change the electronic function **until we find a stable result** (or not).

DFT has its limitations. Nuanced changes in composition (such as through doping) require extremely high computation times.
This should **scale** better on **Quantum Hardware**.

DLR Quantum Computing Initiative (QCI)

- contributes its diverse competencies in quantum research, **from hardware to application**
- Creates suitable environment for **DLR institutes and companies** to work together, focusing on the entire spectrum of QC development
- drives the development of hardware, software and applications for QC in Germany and Europe
- builds up important know-how to **smooth transition to prototype QC use** for its own research
- closely linking research and science with industry and commerce creates the industrial basis and the economic environment for **quantum computers from Germany**
- DLR launched **Innovation Centers** in **Ulm** and **Hamburg**



ExoMatter

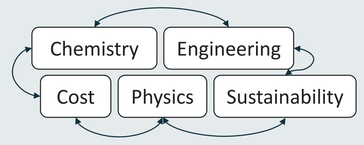
- **Spin-off company/startup,** launched initially at DLR
- Supported by **Helmholtz Enterprise Spin-Off** program
- GmbH established in Munich, **March 2022**
- **6-digit revenues**
- First customers: **Airbus, Audi, Gebrüder Dorfner**

ExoMatter and QCI - The QC Mineral project

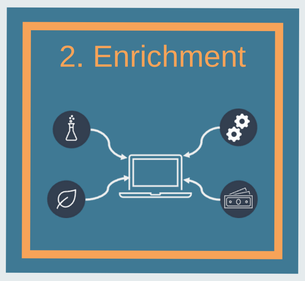
- Collaboration of **DLR Institutes** of **Future Fuels** and **Material Physics**, and companies such as the **DLR-Spinoff ExoMatter**
  - Focus on material design and processes
  - Combining quantum physical calculations in condensed matter with quantum chemical considerations at the atomic level
- Development of **mineral materials** and processes for use in the production of renewable, carbon neutral energy and fuels
- Optimization and development of **novel amorphous solids** (glasses) and glass ceramics
- Rapid **characterization of suitable redox materials** for **solar-powered processes**
- Investigation of **dopants** and **their influence on material properties**
  - Whole series of unit cells has to be simulated
  - In amorphous materials: no clear definition of a suitable unit cell
  - Quantum hardware should make necessary system size accessible

ExoMatter's approach to materials selection

Multi-dimensional analysis of materials properties:
Don't just solve one side of the Rubik's Cube



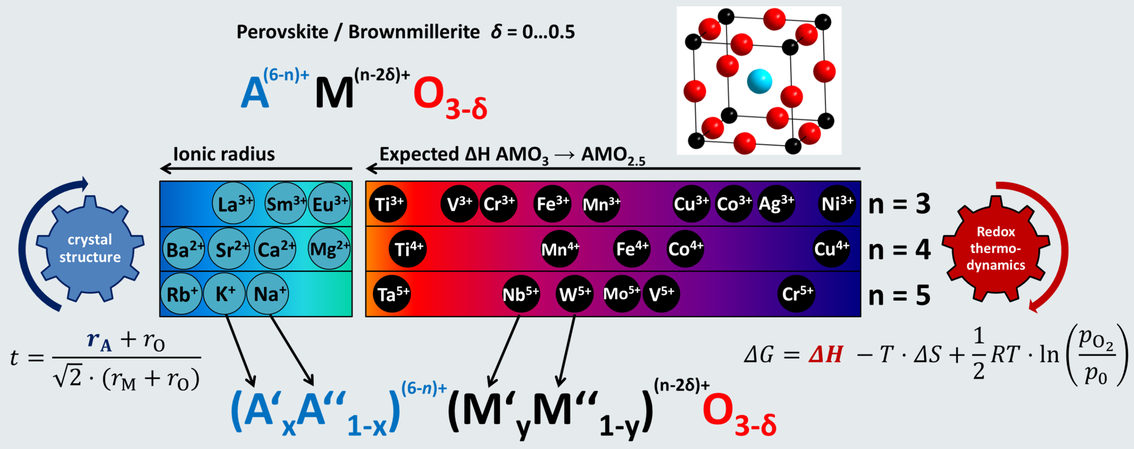
Unify raw data
Scientific databases
Public data
Machine Learning
Custom DFT calculation



Application-specific properties
Chemistry, physics, engineering, cost & sustainability

Enabling decisions
All materials information in one place on a software platform

Case study: Early prototype Perovskite materials for solar fuel production



Target: find novel perovskite materials for air separation

Prototype of ExoMatter code used: Identified perovskite materials with high theoretical fuel conversion efficiency

Systematic materials design was used:
- redox enthalpy tuned via B site ions
- crystal structure modified via A site ions

About one year of experimental work saved!

Vieten et al., Energy Environ. Sci., 12.4, 2019, 1369-1384

UNTERSTÜTZT DURCH DEN IMPULS- UND VERNETZUNGSFONDS VON HELMHOLTZ
DLR
Gründerland Bayern
Bayerisches Staatsministerium für Wirtschaft, Landesentwicklung und Energie