AUTOMATION, DATA DRIVEN AND MACHINE LEARNING METHODS IN COMPUTATIONAL MATERIALS DESIGN

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### Outline

- Automated DFT simulations – digital materials design
- Data-driven microstructure generation – virtual microstructure design
- Data-driven materials science – automated extraction of semantic relations
Automated DFT simulations
Modelling SOFC anode aging

Problem
- Ni-YSZ\(^1\) anode degradation qualitatively understood: Ni grains coarsen over time: performance degradation
- Need for quantitative lifetime prognosis > 3000 h, but no validated accelerated lifetime tests

Research objectives:
With combined experimental and simulative multiscale modelling
- Understand relation between anode microstructure evolution and degradation rate
- Propose optimized microstructure
- Focus on interoperability in modelling chain

\(^1\) Yttria-stabilized zirconia
Automated DFT simulations
AiiDA at Bosch

**AiiDA** – Automated Interactive Infrastructure and Database for Computational Science
- Job manager
- Workflow manager
- Database

**Origin of AiiDA**
- Joint project between THEOS group / MARVEL Center at EPFL and Research and Technology Center NA at Bosch
- Now Open source project
- Bosch is still actively contributing to its further development

Shown **tools** have been interfaced with each other to obtain **various properties**

Visualization
- Phase diagrams
- DFT code: energies, forces, electronic structure

Genetic algorithms for ground state comp.
- Genetic algorithms
- Ground state comp. esp. for alloys

LSF scheduler
- Job scheduler for HPC
- Error management

**BOSCH HPC**

GA

ASE

ATAT

LSF scheduler

VASP

pymatgen

Phonopy

custodian

**Shown tools have been interfaced with each other to obtain various properties**
Automated DFT simulations

Use case for linked / coupled workflows

Output on atomistic scale

- Surface energies of Ni with different surface orientations: material parameter 1 for extended phase field simulation
  - Validation with experimental data (weighted average)
- Adsorption energies of Ni / H₂ on Ni surface: input for calculation of diffusion constants
  - Diffusion constants: material parameter 2 for phase field

Current status workflow and linking

- Manual data transfer to partners required
- Workflow not automated
- Open simulation platform would enable process automation

1 Instead of total diffusion, volume and surface diffusion calculated individually at HS Karlsruhe
### Outline

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Data-driven microstructure generation

Speed-up in materials development

Motivation

- Properties of heterogeneous materials depend strongly on microstructure
- Optimizing microstructure by trial-and-error very lengthy and expensive because of the long experimental chain (sample manufacturing, analyses, measurements)
- Explore potential of data-based methods for accelerating materials development on micro-scale.

Use cases

- Fuel cell anode (SOFC) porous Ni-YSZ composite
- Ceramic composite material glass particles in precursor matrix
- Martensitic steel nested grain structure
- Short glass fiber reinforced thermoplastics (SFRT)

Source: KIT, PIP KerSOLife100
Funding No. 03ET6101A
Data-driven microstructure generation
Current status: process of materials development

Manufacturing process → Sample
- Sample manufacturing
- Measurement
- 3D analysis

Effective properties:
- Conductivity
- E-modulus
- Strength
- ...

Simulation
- Microstructure simulation
- synthetic generation
- use observed microstructure directly
- generate realistic microstructures using stochastic geometry
- adjust microstructure characteristics

Statistical descriptors
- Volume
  - Perc: 43.9% → 30%
  - Interface area: 41/µm² → 12/µm²
  - # particles: 10
  - Grain size (GS): 34 µm → 90 µm
  - GS Std. Dev.: 48 µm → 168 µm

Arrow thickness: Throughput capacity
Data-driven microstructure generation
Perspective: use potential of data-based approaches

Limitation of current approach
- Many manufactured samples required for statistical microstructure reconstruction
- Simulations do not provide design rules for microstructure optimization → trial and error

Idea of data-driven microstructure generation
- Predict effects of variations in microstructure
- For realistic microstructures: need for data-based generator

- Virtual microstructure design can speed-up and reduce costs of materials development significantly
- Marketplace platform beneficial for linking of tools and use of database

Step 1: Generate virtual twin

Step 2: Parameter variations

1 using databases and/or AI methods with data of previously/virtually reconstructed microstructures
2 Source: Westhoff et al., Computational Materials Science 126 (2017) 453–467, Ulm University, Institute of Stochastics
4th Workshop on Interoperability in Materials Modelling
Automation, data driven and ML methods in computational materials design

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Data-driven materials science
Access unstructured data, uncover hidden knowledge and make predictions

Project scope
- Automated knowledge based analysis of literature, patents and websites

Advantages
- Vast amounts of available unstructured data and knowledge made accessible
- High efficiency by structured data compared to pdf-document collection
- Hidden knowledge can be extracted, new knowledge can be predicted.

Text mining: From vast amounts of unstructured data to a structured knowledge
Data-driven materials science
Application: text mining for magnetic materials

Objective

- Efficient extraction of design rules for hard magnets from publications, patents and websites

Results

- Text mining method from drug discovery transferred to material science w/ external partner
- Structured hard magnets knowledge created as ontology for semantic text processing
- ~10,000 magnetic material properties from more than 2 million publications extracted
Data-driven materials science
Combination with other data sources

- Integration of different data sources into a data warehouse to unify access
  - Literature data from text mining results
  - Crystal Structure Databases: ICSD\textsuperscript{1}, COD\textsuperscript{2}, Pearson\textsuperscript{3}
  - Ab-initio databases: Materialsproject, AFLOW\textsuperscript{4}, OQMD\textsuperscript{5}

- Specific hard-magnetic data sources
  - Ab-initio results from LMTO\textsuperscript{6} calculations (Prof. Elsässer, FhG IWM)
  - Results from own experiments

1 Inorganic Crystal Structure Database, \textsuperscript{2} Crystallography Open Database, \textsuperscript{3} Crystal Structure Database For Inorganic Compounds, \textsuperscript{4} Materials Property Database, \textsuperscript{5} Open Quantum Material Database, \textsuperscript{6} Linear muffin-tin orbital (Ab-initio method, alternative to DFT)