## Programme June 23rd 2021

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<th>Time</th>
<th>Speaker</th>
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- **Dr. Marcel Sluiter** (Associate professor, Materials Science and Engineering, 3mE, Delft University of Technology and visiting professor in the Department of Electromechanical, Systems and Metal Engineering, Faculty of Engineering and Architecture, Ghent University)
Materials Science DATA

ICSD icsd.products.fiz-karlsruhe.de

4TU ResearchData: data.4tu.nl/info/en/
MatNavi: mits.nims.go.jp/en/
Materials Cloud Archive: archive.materialscloud.org

Theory:
aflow-ML
materials project
Nomad
Oqmd
Natural Language Processing in Materials Science

- Materials Science literature very extensive and scattered
- Experimental measurement methods (very many)
- Computation/simulation (very many)
- Material processing/prep./prior history crucial

Olivetti et al. doi: 10.1063/5.0021106
Classification in Materials Science

Image processing: microstructure recognition?

(a) quiz 1

(b) quiz 2

Larmuseau et al. doi: 10.1016/j.scriptamat.2020.10.026
Classification in Materials Science

Larmuseau et al. doi: 10.1016/j.scriptamat.2020.10.026
Material properties complex function of composition (processing etc.) actual alloys never “binary” or “ternary”

Martensite Start temperatures of steel as function of composition (15 alloying elements)
Regression in Materials Science

Training data vs test data for KNN $n_{\text{loops}}=50$

Comparison thermodynamics-based model (brown) vs ML model developed in the present work (green).

Ramahan et al. doi: 10.1007/s11661-019-05170-8

TUD/MSE MS43205 course project: C. Martinez Fornos, S. Liu, S. van ’t Sant
Data from wwwphase-trans.msm.cam.ac.uk/map/data/materials/Ms_data_2004.html
Materials Discovery via AI in Materials Science

Theory databases
- DFT
- Force fields
- Thermodynamic

Combinatorial libraries
- Structural and functional libraries
- Property prediction
- Processing impacts
- Non-equilibrium maps

Imaging libraries
- Atomic-scale imaging
- Microstructures
- Functional imaging
- Multi-modal characterization

Integration
- ML tools
- Feature generation
- Bayesian frameworks
- Statistical models

Active learning
- Experiment feedback

Error corrections
- New calculations

Predictions use as priors

Expand libraries

Guidance
- Predictions
- Optimization

Vasudevan et al. doi:10.1557/mrc.2019.95
Searching for new high $T_c$ superconductors

Schmidt et al. doi:10.1038/s41524-019-0221-0
Artificial Intelligence in Materials Science

Natural Language Processing

Classification & Regression

Materials Discovery & Design
(composition/processing(thermomechanical)/nanostructured/metamaterials)

"enhanced" experimental measurements (e.g. EBSD) camera software, TEM: Image reconstruction (e.g. defocus-image modulation)

constructing with materials, optimal shape, optimal local properties 3d printing - unique ability of vary composition & properties in one continuous piece
AI in Materials Science

improved design: functional structures/constructions
Miguel Bessa

improved process: utilization/monitoring/production
Dimitrios Zarouchas

improved materials: physical simulation/fundamental understanding
Menno Bokdam & Ondrej Rokos
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