4TU.HTM

Artificial Intelligence in Materials Science

June 23rd 2021 session

Marcel Sluiter

TU Delft & Ghent University

Programme June 23rd 2021

	Introduction & chair **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)
15.00 - 15.30	**Miguel Bessa (TU Delft)** *Spider web nanomechanical resonators with Bayesian optimization*
15.30 - 16.00	**Dimitrios Zarouchas (TU Delft)** *Adaptive prognostics for remaining useful life of aerospace structures utilizing fused health monitoring data and machine learning*
16.00 - 16.30	**Menno Bokdam (UTwente)** *On-the-fly machine learning force fields with near first principles precision: Predicting phase transitions in complex solids*
16.30 - 17.00	**Ondrej Rokos (TU/e)** *Learning constitutive models in multiscale modeling of materials*

Materials Science **DATA**

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

ICSD icsd.products.fiz-karlsruhe.de

4TU ResearchData: data.4tu.nl/info/en/
MatNavi: mits.nims.go.jp/en/
Materials Data Repository: www.nist.gov/programs-projects/materials-data-repository
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

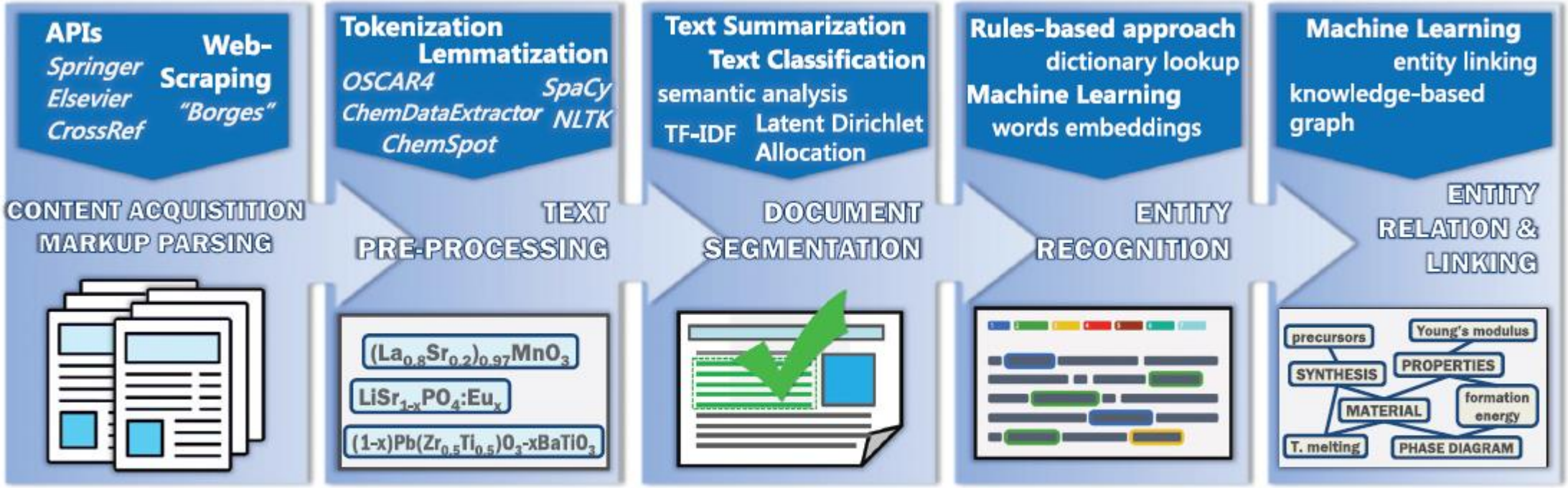
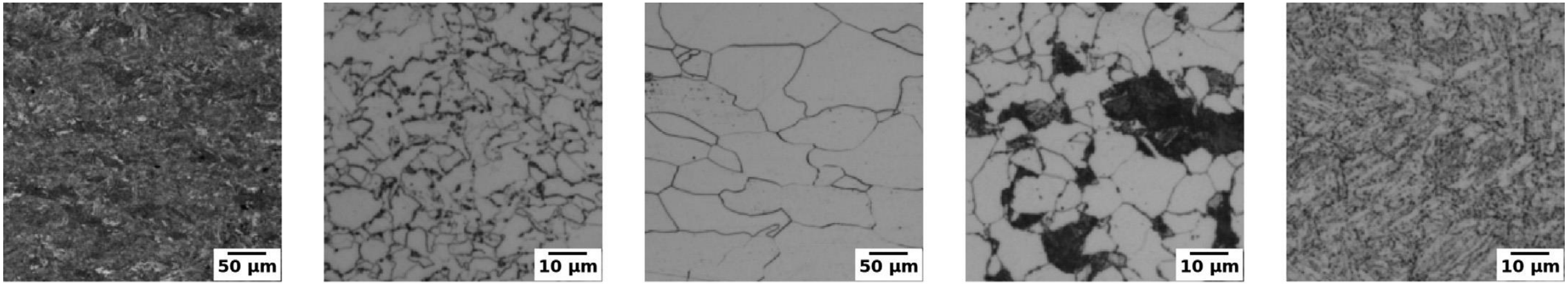


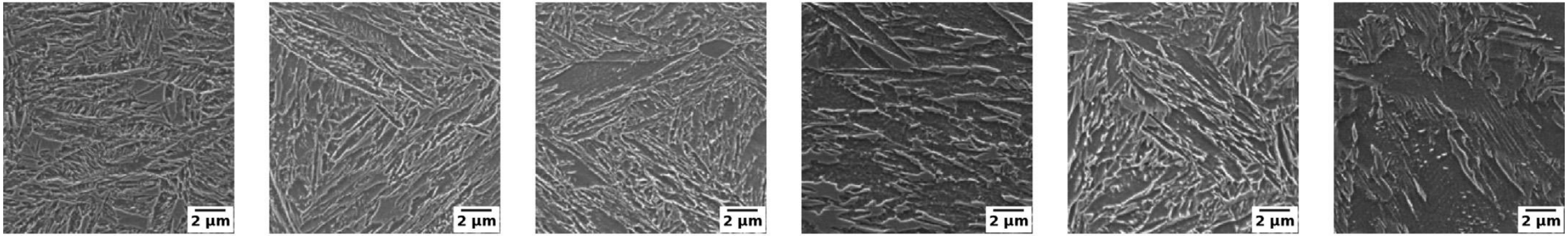
FIG. 2. Schematic of NLP including examples of tools and models at each step. It is visible that most natural language extraction follows similar approaches: (1) acquiring relevant text resources, (2) processing the text into individual terms (also known as tokenization), (3) document segmentation and paragraph classification, (4) recognizing tokens as classes of information, (5) entity relation extraction, and (6) named entity linking.

Classification in Materials Science

Image processing: microstructure recognition?



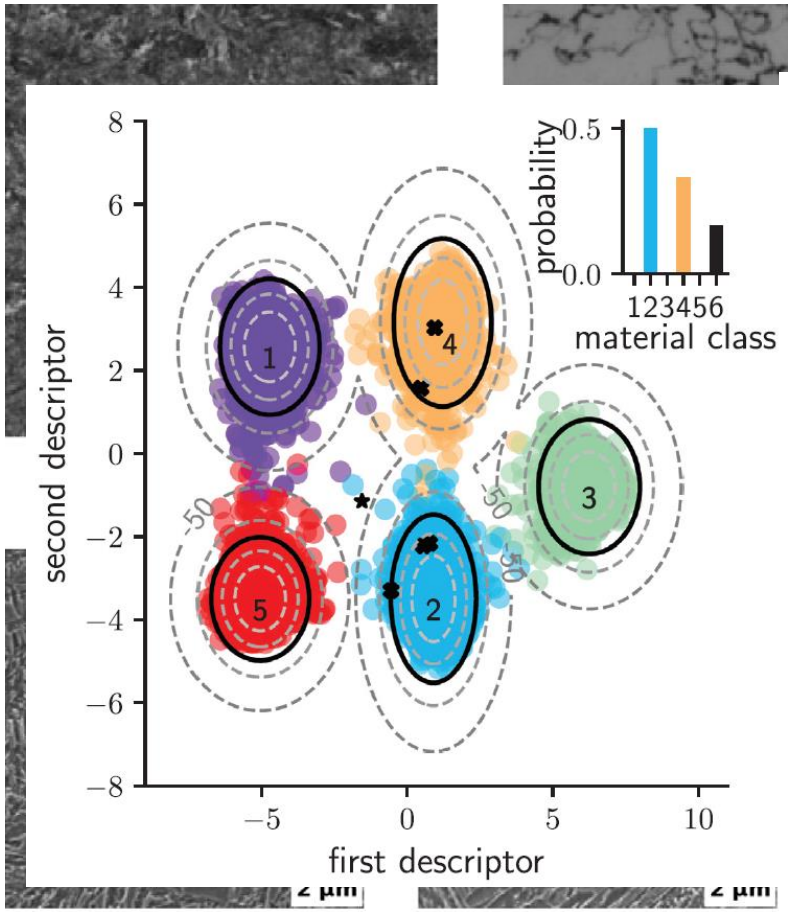
(a) quiz 1

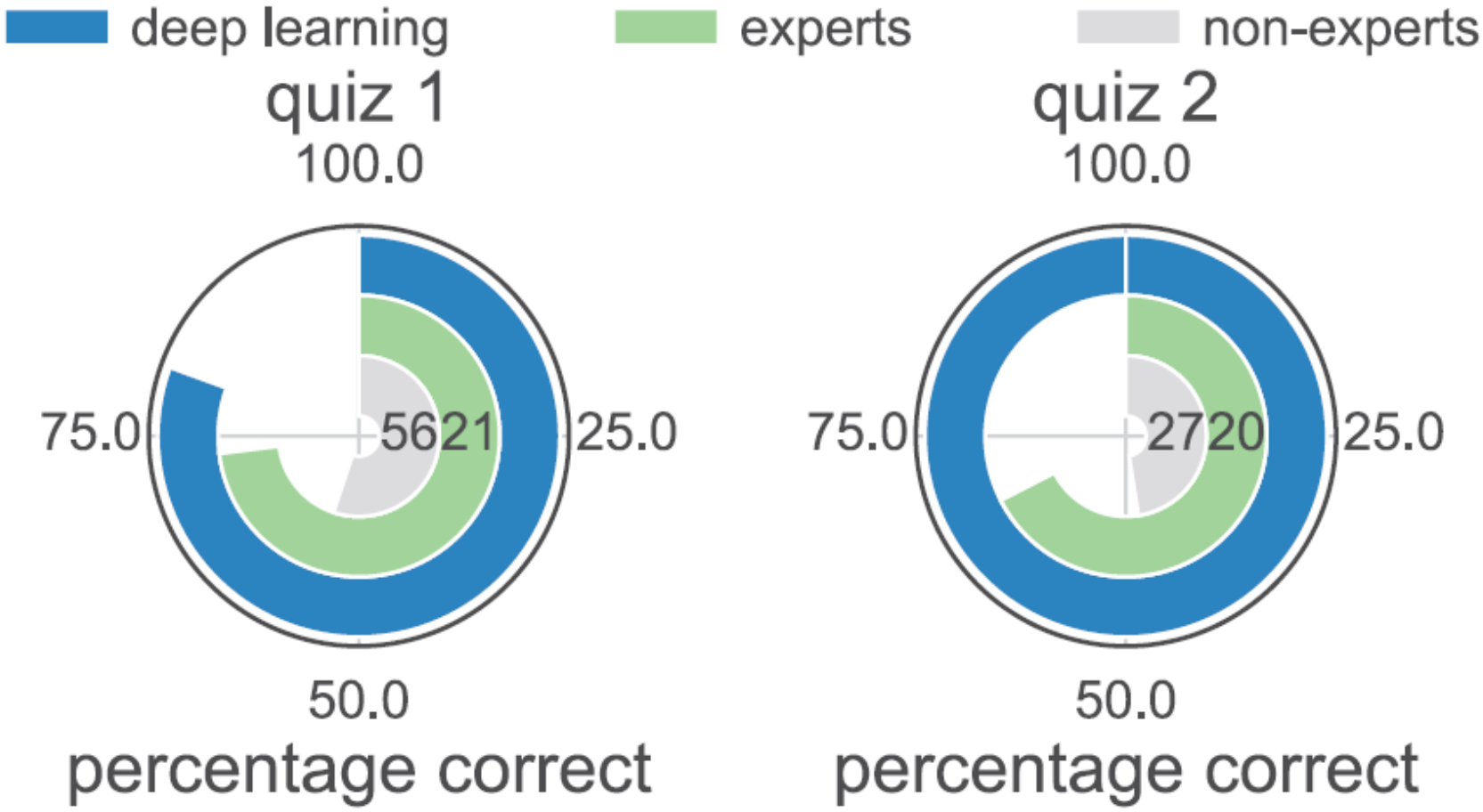


(b) quiz 2

Larmuseau et al. doi: 10.1016/j.scriptamat.2020.10.026

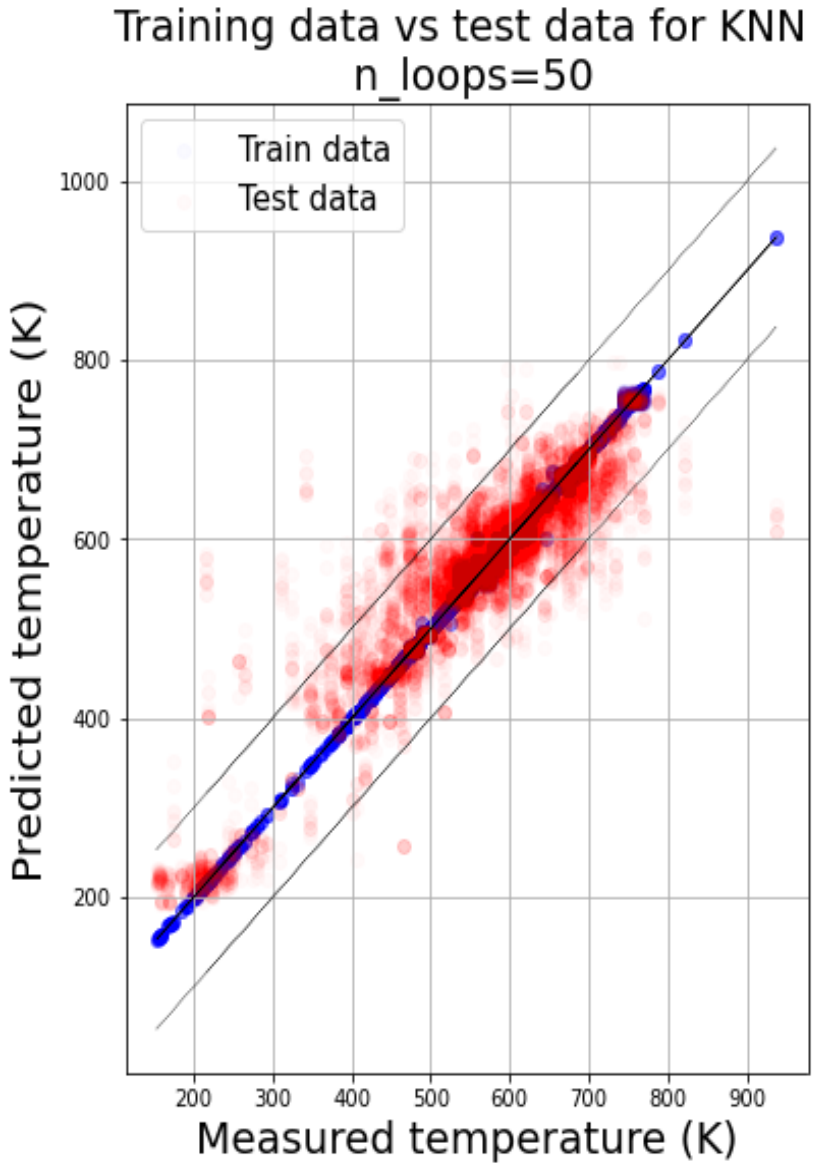
Classification in Materials Science





Larmuseau et al. doi: 10.1016/j.scriptamat.2020.10.026

Regression in Materials Science

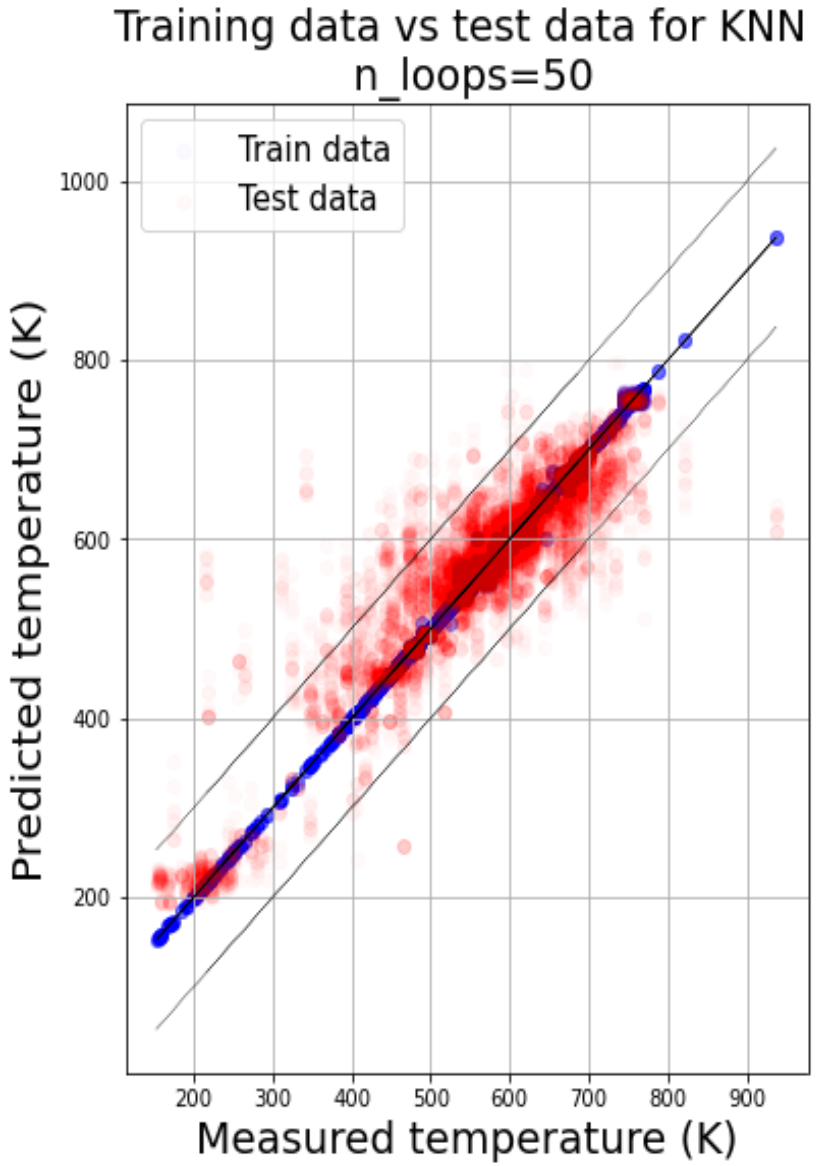


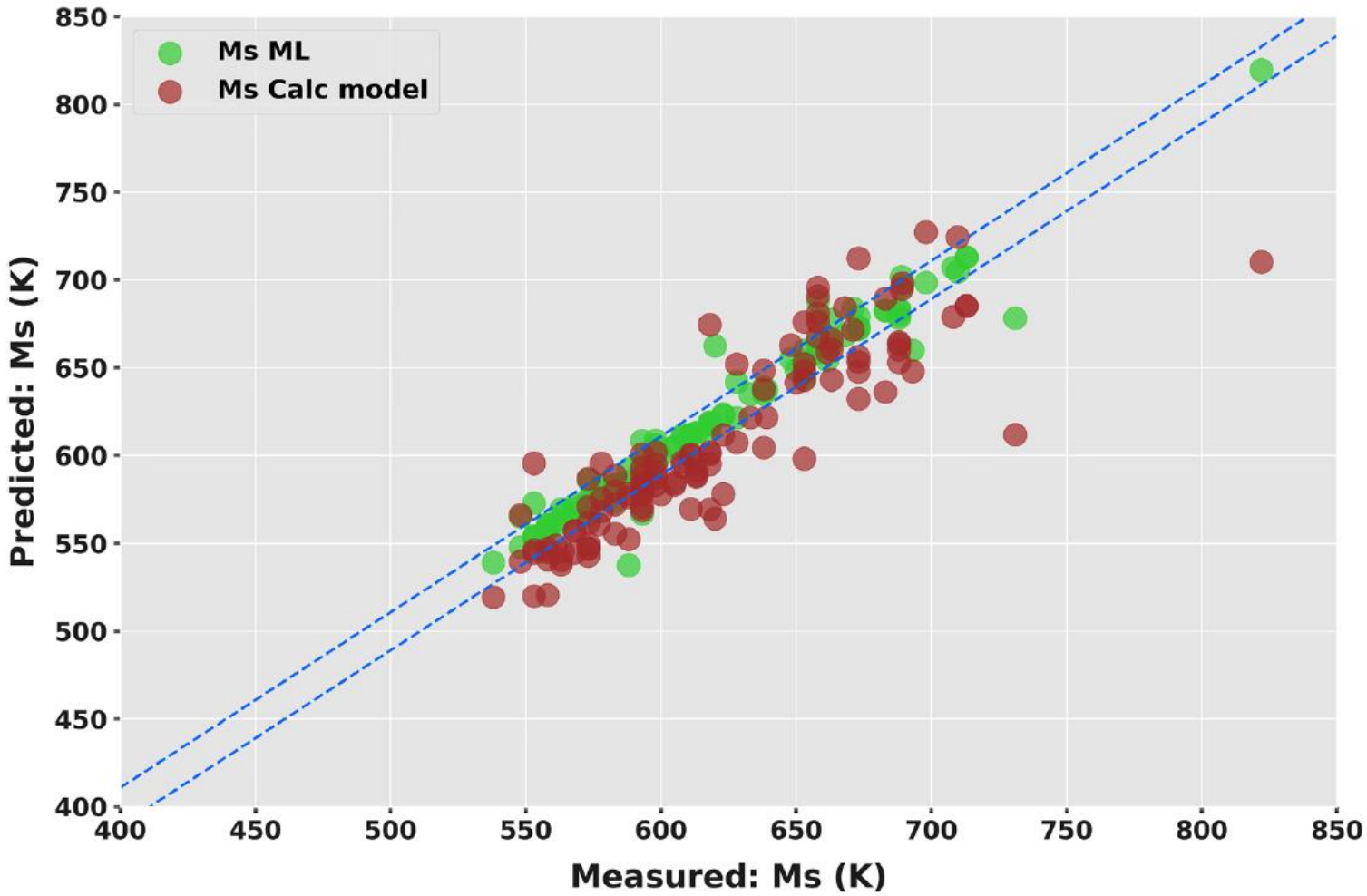
Material properties complex function of composition (&processing etc.)
actual alloys never “binary” or “ternary”

Martensite Start temperatures of steel as function of composition (15 alloying elements)

TUD/MSE MS43205 course project: C. Martinez Fornos, S. Liu, S. van ’t Sant
Data from www.phase-trans.msm.cam.ac.uk/map/data/materials/Ms_data_2004.html

Regression in Materials Science





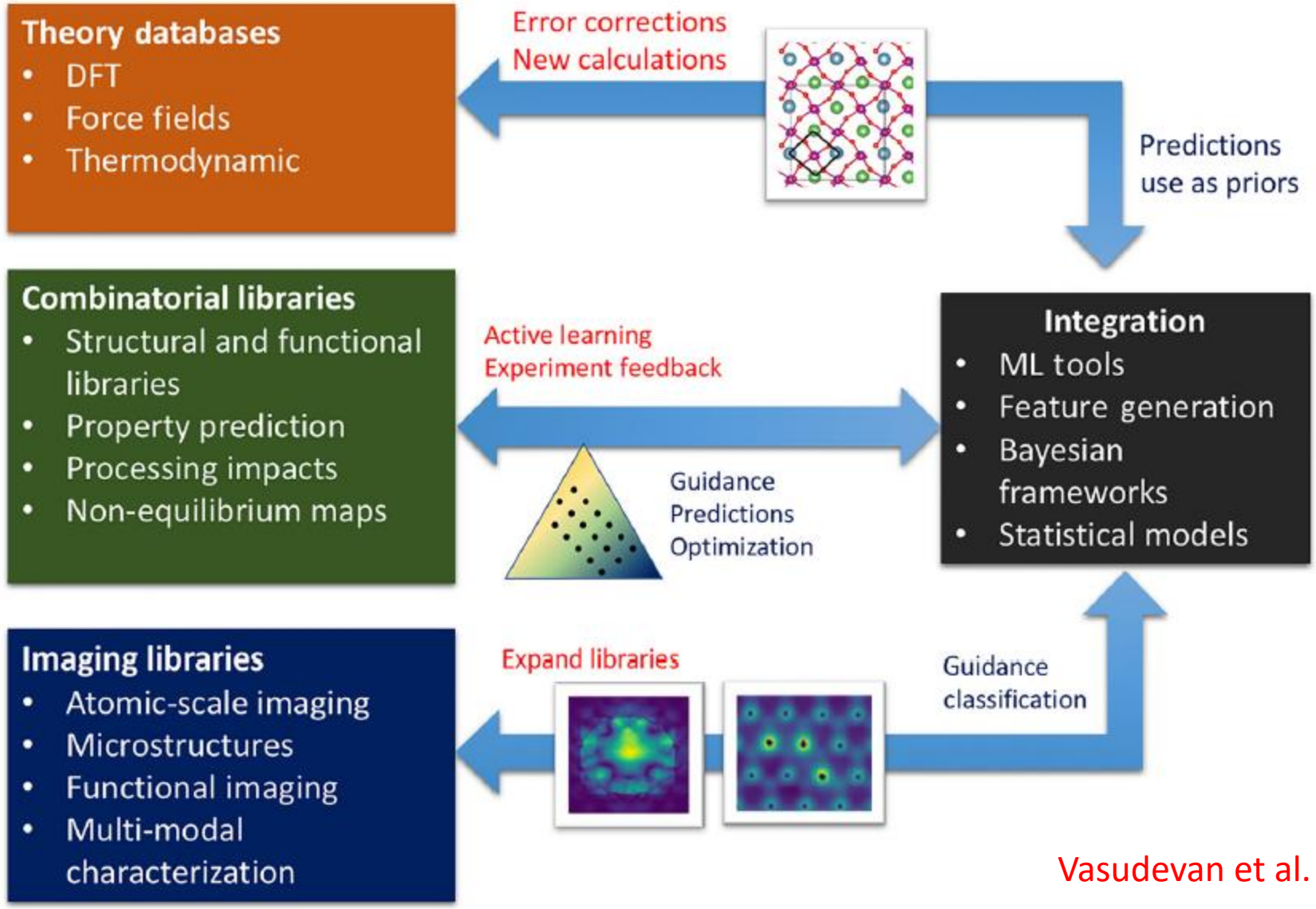
Comparison thermodynamics-based model (brown) *vs* ML model developed in the present work (green).

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

TUD/MSE MS43205 course project: C. Martinez Fornos, S. Liu, S. van ’t Sant

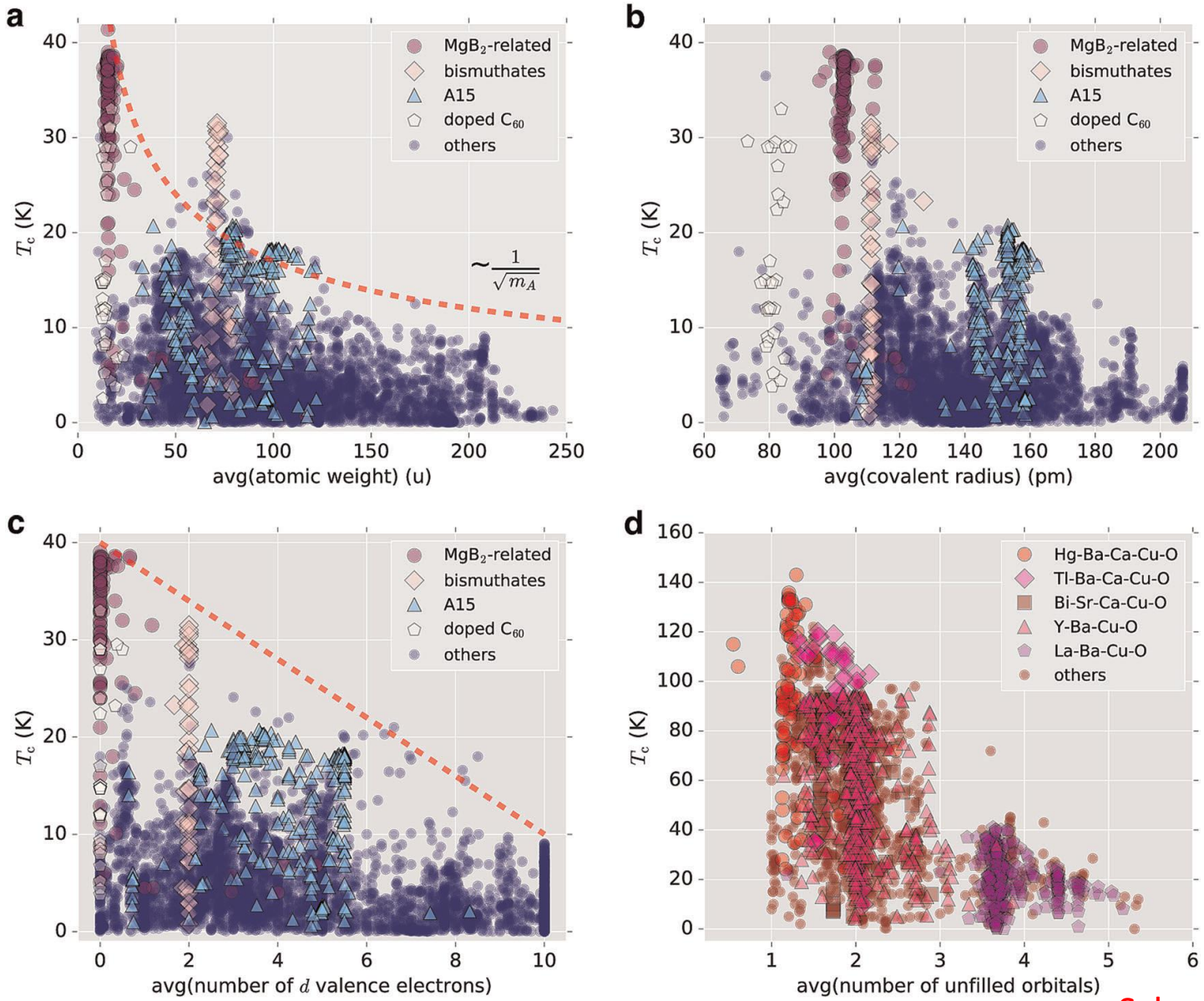
Data from www.phase-trans.msm.cam.ac.uk/map/data/materials/Ms_data_2004.html

Materials Discovery via AI in Materials Science



Vasudevan et al. doi:10.1557/mrc.2019.95

Materials Discovery via AI in Materials Science



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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