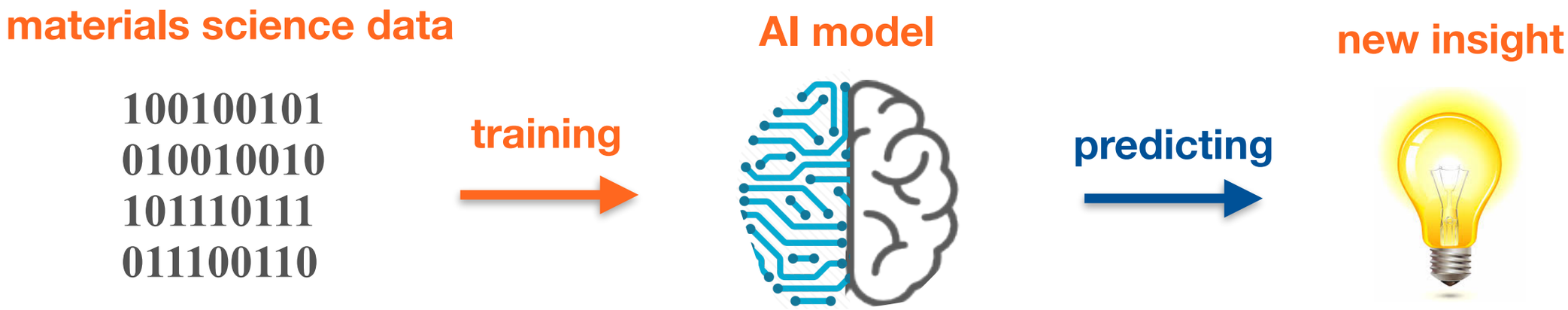
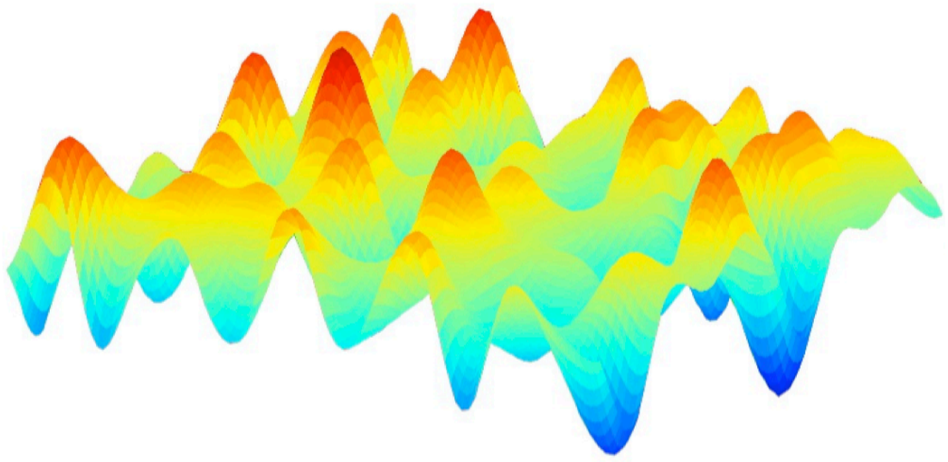
Artificial intelligence and data-driven material and device engineering



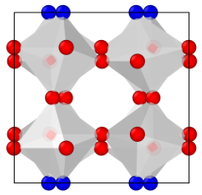
Accelerating discovery in materials science:

- data analytics
- pre-screening
- materials design
- device tuning and optimization
- guiding experimental data collection

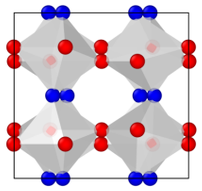
processing-structure-property-function relationships



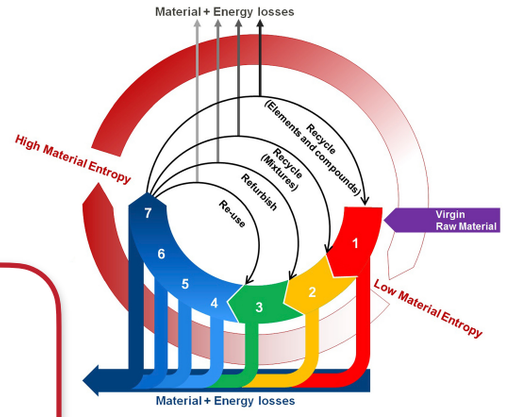
Materials Informatics Laboratory at UTU



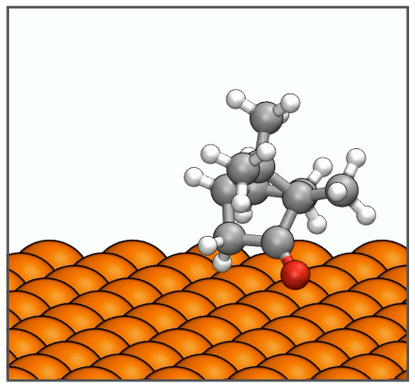
substitutional engineering



critical materials recovery



interface structures



AoF: LearnSolar, DeeperMaterials

Materials design

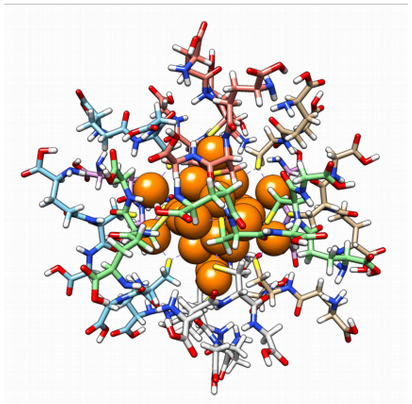
AoF: AIMSS

Organic/inorganic interfaces

AoF: SmartCycling

Circular economy and recycling

materials for devices



AoF: Brilliant-AI

Solar cells, health, sensors, climate

AoF: AI-Lignin

Bio-derived materials

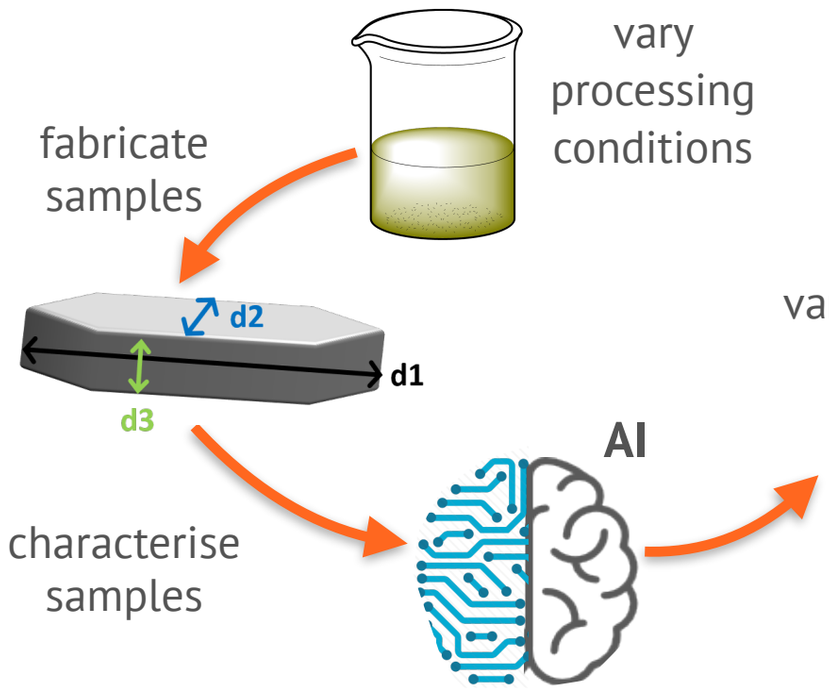
lignin biorefinery optimisation

Applying AI to refine experiments

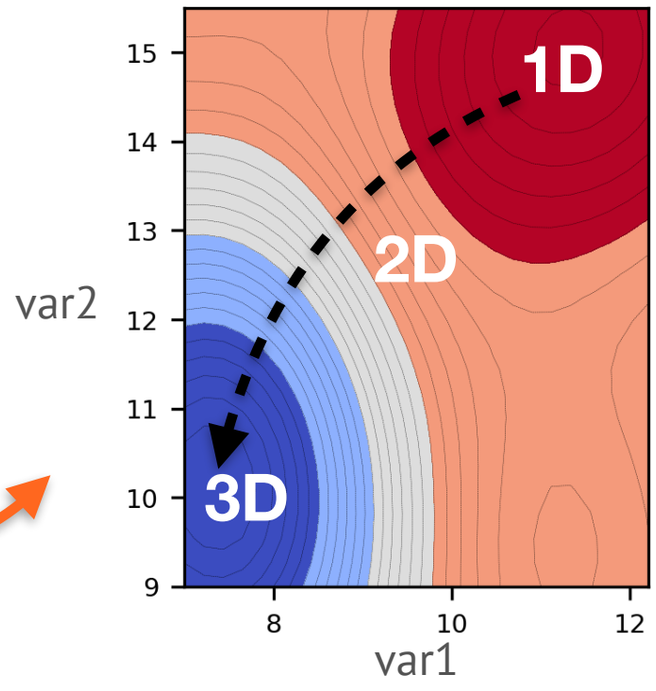
Bayesian Optimization **guides experimental data collection** to develop **predictive models** (possibly high-dimensional) and **optimize target properties,** while conducting **as few experiments as possible.**

EXAMPLE: particle morphology engineering (17 samples)

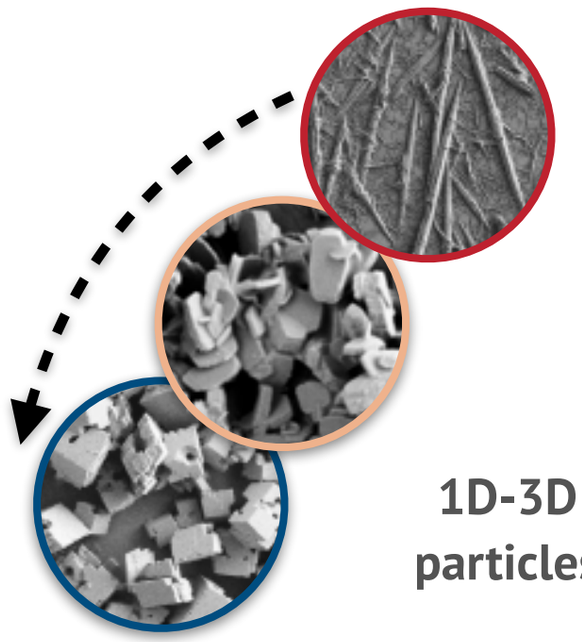
1. conduct experiments



2. map material property



3. designer materials



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AI-driven optimal outcomes in SmartBIO

Potential applications in SmartBIO

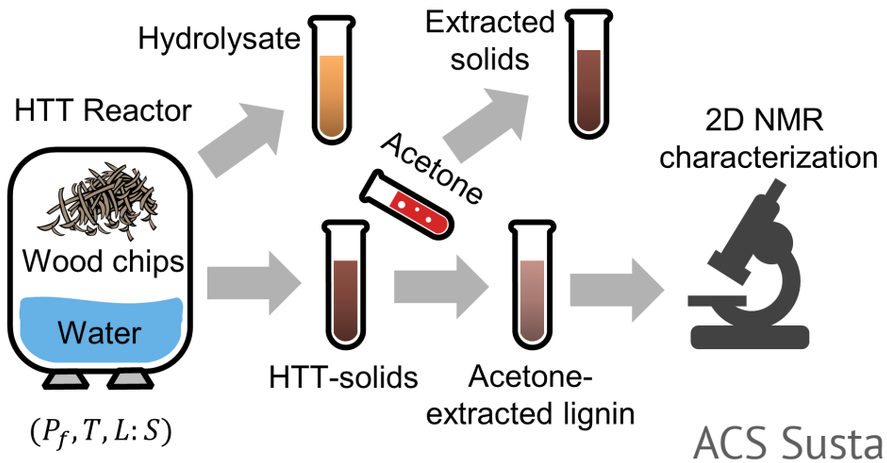
Materials: multi-objective optimisation of bio-derived materials

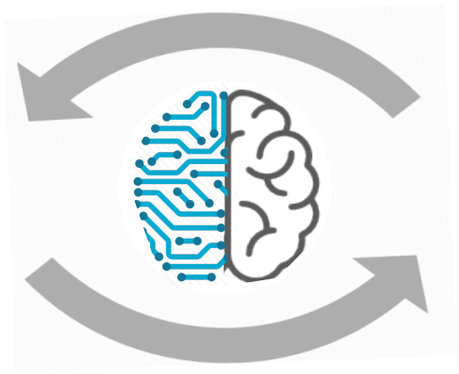
Processes: optimisation of synthesis / functional processes

Devices: device performance optimisation and customisation

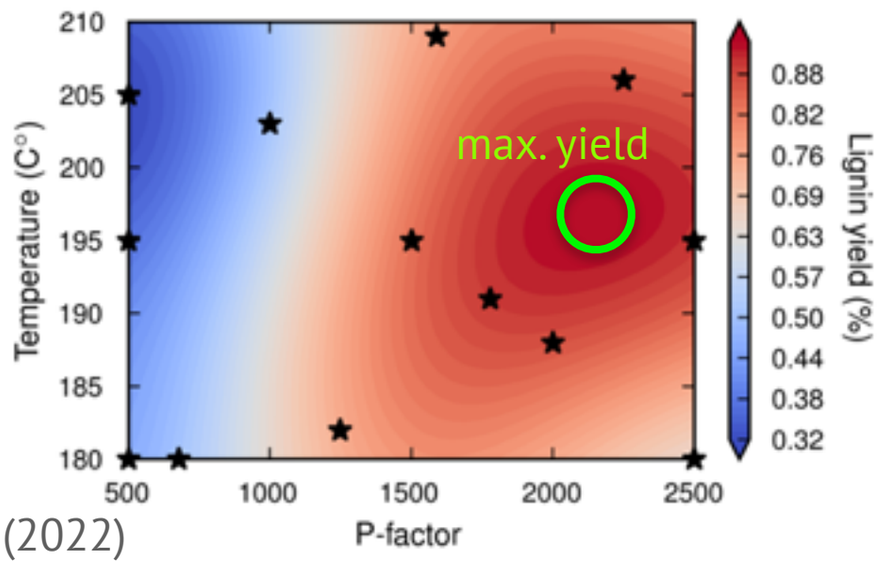
EXAMPLE: material process engineering (21 samples)

Variables: P-factor, temperature
Target property: Lignin yield





Predictions and optimisation



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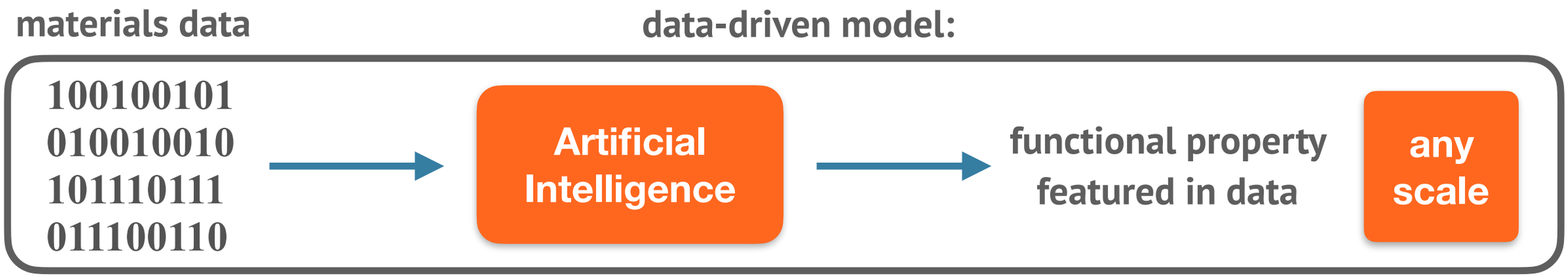
Why data-driven models?

milica.todorovic@utu.fi



Works with many types of data:

- Material properties (composition, shape, weight…)
- Processing conditions (flow, temperature, pressure…)
- Device parameters (layer thickness, dimensions…)
- Instrument settings

Advantages:

- Sample-efficient and guided data collection (Design of Experiments)
- Yields easily interpretable correlations between target properties and experimental variables.
- Allows multi-objective optimisation