AI-driven design of materials (Highlight E)
The mission of FCAI Highlight Program E is to develop AI technology for accelerated materials design and characterization.

Program objectives
Materials are the foundation of technological developments that shape our modern society. Their continuous development enables new applications and products, while the discovery of novel materials addresses such societal challenges as clean energy production, global prosperity, health and wellbeing. To meet these challenges, this highlight will develop AI technology for materials design and characterization.

Methodologies
We use and adapt a variety of machine learning and AI tools
- Dimensionality reduction
- Bayesian optimisation
- Simulator-based inference
- Kernel ridge regression
- Gaussian process regression
- Decision trees and random forests
- Neural networks (convolutional, deep tensor)
- Encoder-decoder neural networks

Research results

Artificial intelligence for spectroscopy: Deep neural networks predict molecular excitation spectra with 97% accuracy in spectral weight and 0.2 eV in peak positions [1].

Active learning in materials synthesis (collaboration with FinnCERES flagship): BOSS engineered the shape of tannic acid nanoparticles to determine which growth conditions produce the desired target shapes (1D, 2D, or 3D). With only 9 experimental data points (pink circles), BOSS visualised the dependence of the nanoparticle shape on the growth conditions pKa (chemical base strength) and pH (solution acidity) in an intuitive map.

Bayesian Optimisation for Structure Search (BOSS) [2]
BOSS predicts the adsorption site and geometry of organic molecules on inorganic surfaces efficiently (i.e. with a minimum of costly quantum mechanical calculations). The BOSS prediction of camphor on copper show in the figure is now being validated experimentally with scanning probe microscopy.


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