FCAI Finnish Center for Artificial Intelligence

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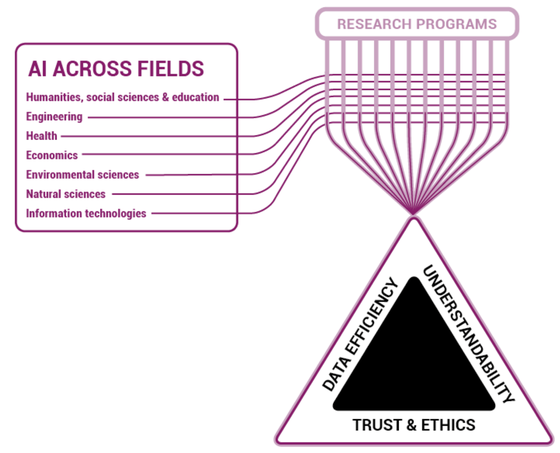
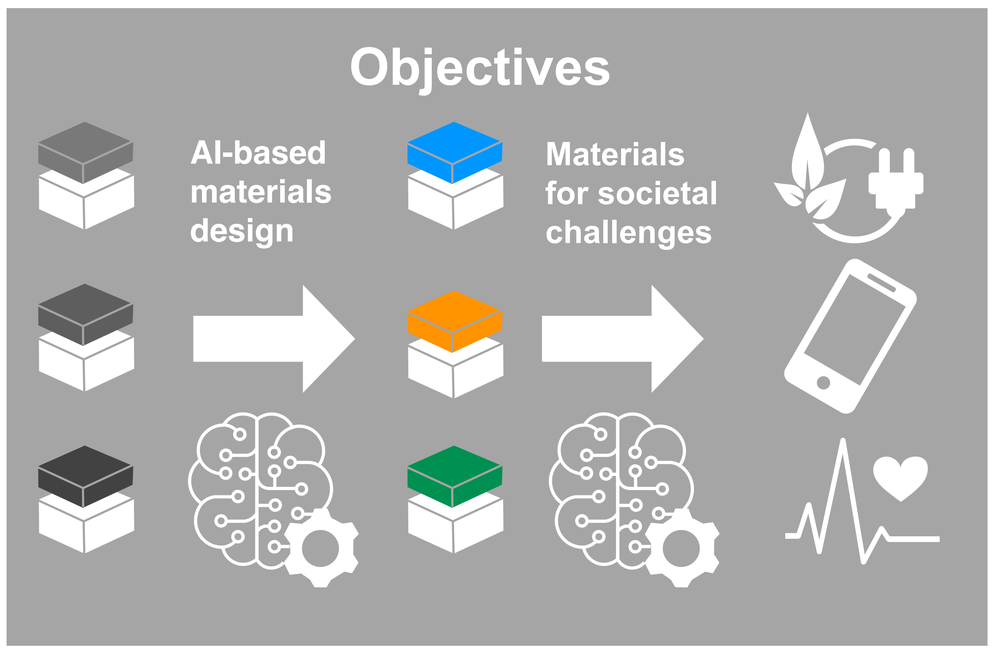
AI-driven design of materials (Highlight E)

The mission of FCAI Highlight Program E is to develop AI technology for accelerated materials design and characterization



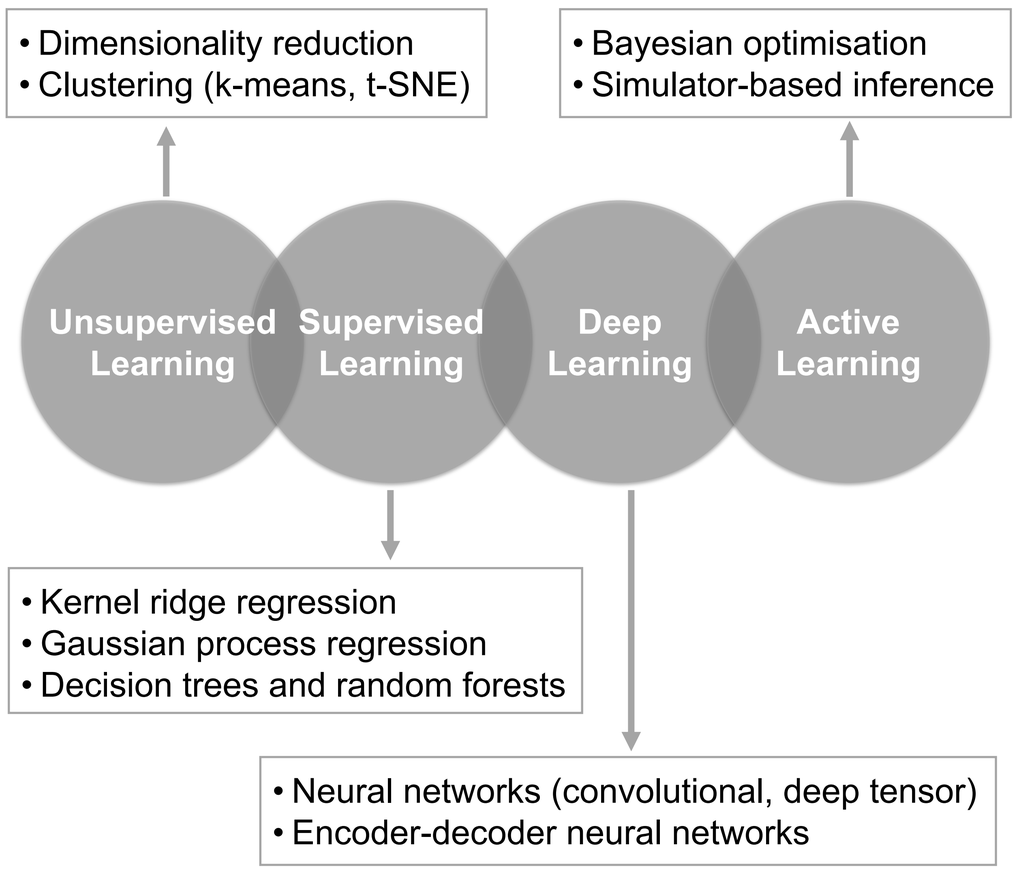
Program objectives

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.



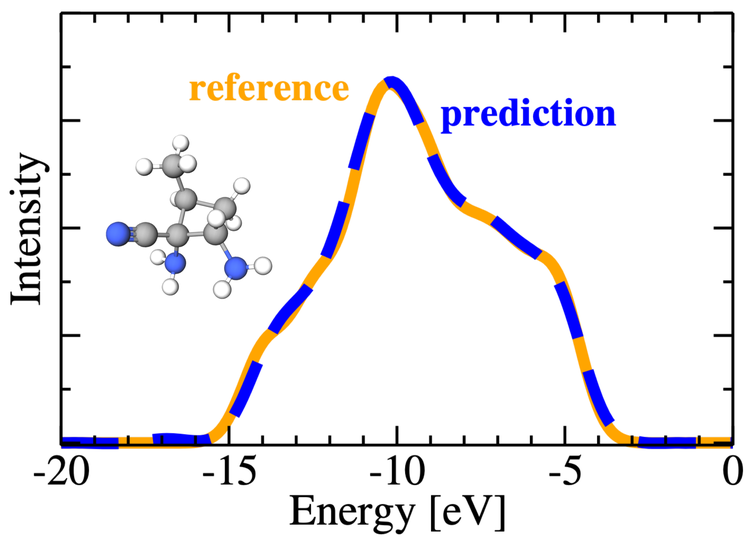
Methodologies

We use and adapt a variety of machine learning and AI tools

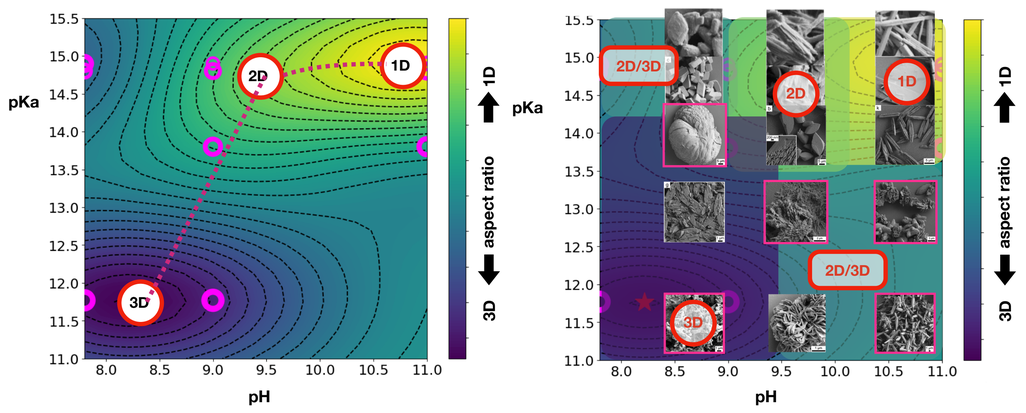


Research results

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].

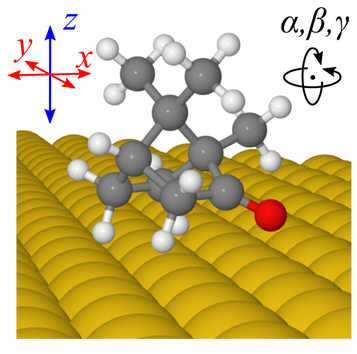


Active learning in materials synthesis (collaboration with FinnCERES flagship): BOSS engineered the shape of tannic acid nanoparticles to determine which growth conditions produce the desired target shapes (1, 2, or 3D). With only 9 experimental data points (pink circles), BOSS visualised the dependence 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.



[1] K. Ghosh, A. Stuke, M. Todorović, P. B. Jørgensen, M. N. Schmidt, A. Vehtari and P. Rinke, Adv. Sci. 6, 1801367 (2019)
[2] M. Todorović, M. U. Gutmann, J. Corander and P. Rinke, npj Comp. Mat. 5, 35 (2019)

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FCAI is a nation-wide competence center for Artificial Intelligence in Finland, initiated by Aalto University, University of Helsinki, and VTT Technical Research Centre of Finland. FCAI is one of the six Academy of Finland Finnish flagships.

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