FCAI Finnish Center for Artificial Intelligence

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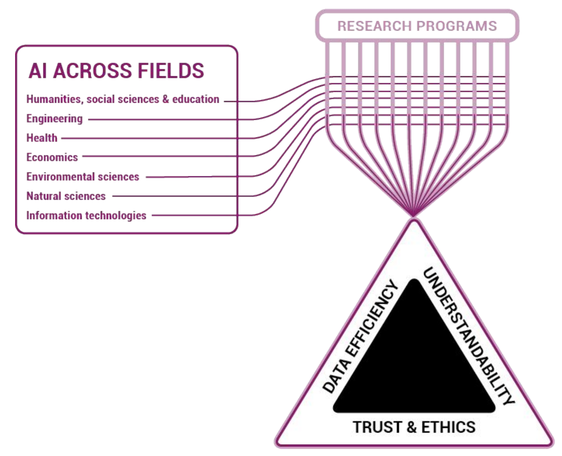
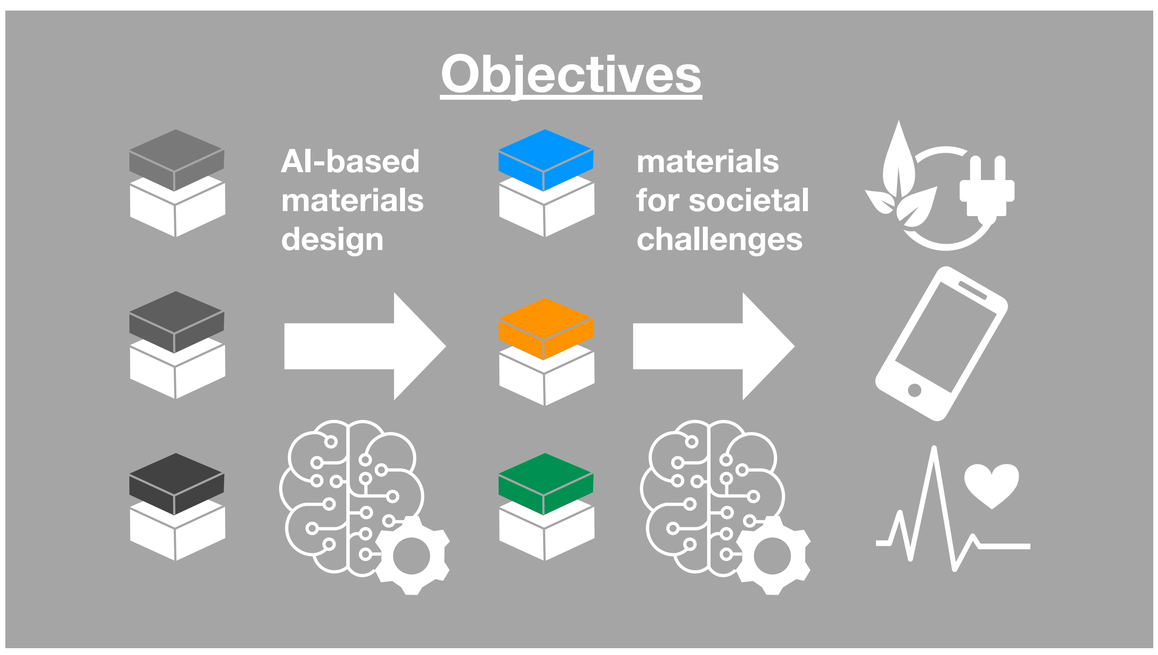
AI-Driven design of materials (Highlight E)

Our mission is to develop AI technology for accelerated materials design and characterization



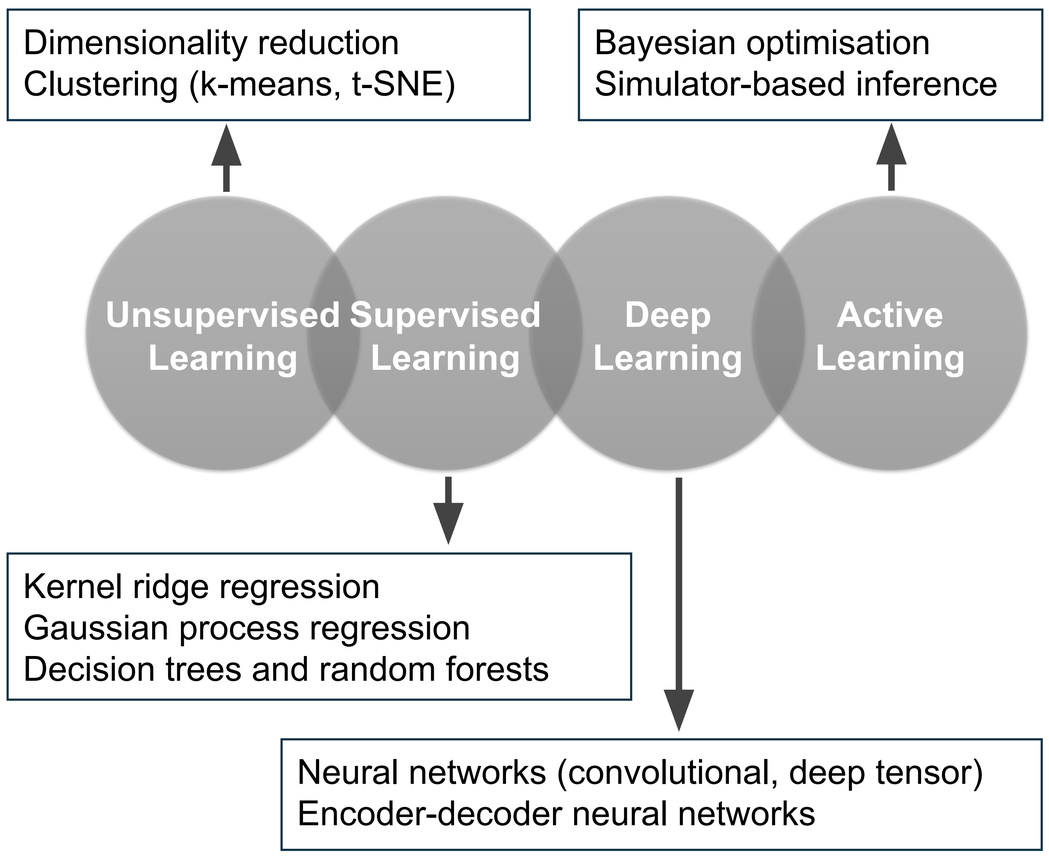
Program objectives

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 is developing AI technology for materials design and characterisation.



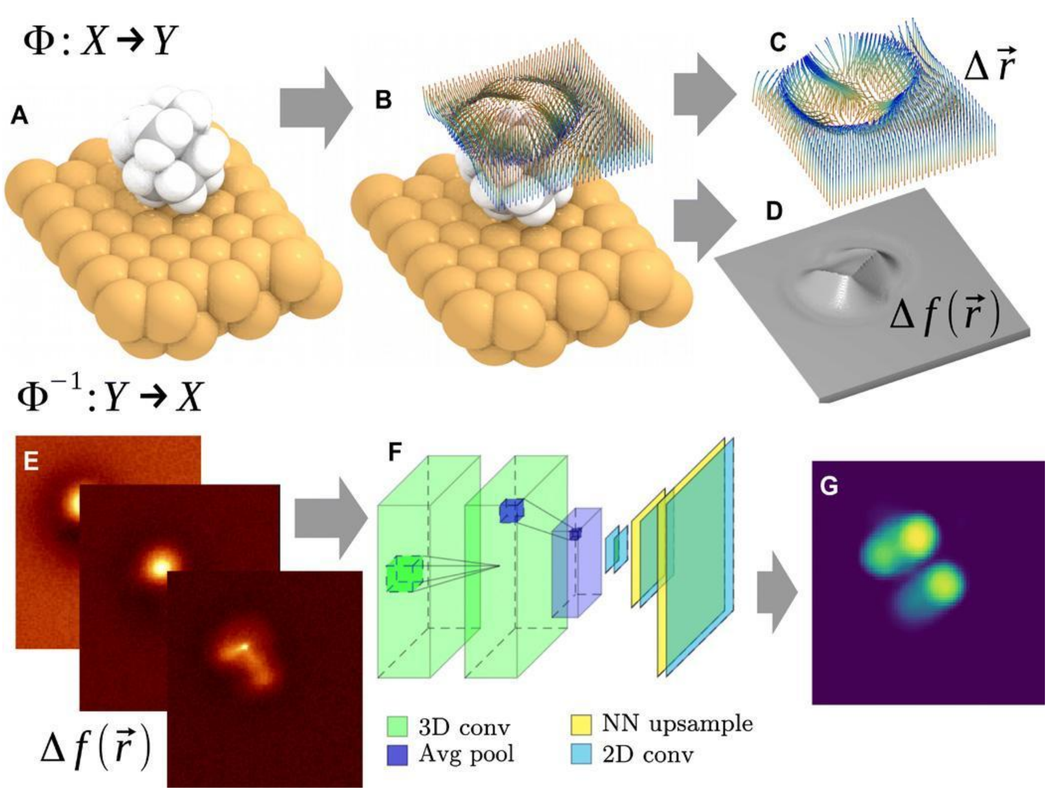
Methodologies

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

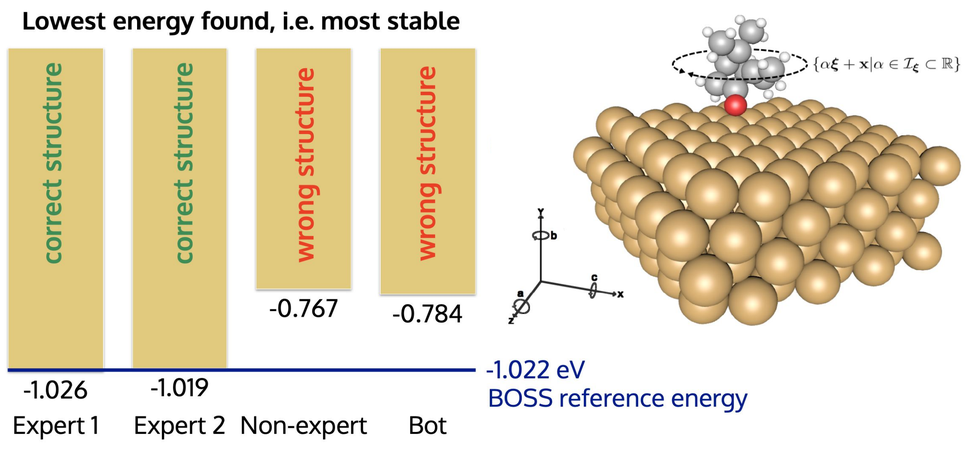


Research results

Automated structure discovery in atomic force microscopy: Atomic force microscopy (AFM) is the primary experimental technique to characterise molecules and materials with atomic resolution. A breakthrough was achieved by combining AFM with a newly developed deep learning neural network infrastructure (see image below), that for the first time unveils the atomic structure of bulky molecules, whose structure cannot be inferred from AFM images alone [1].



Towards AI-assisted decision making: We implemented a Projective Preferential Bayesian Optimization (PPBO) scheme to include the *human in the loop* in complex materials optimisation tasks. Our PPBO tested on the adsorption structure of a camphor molecule on the copper surface (right) encodes expert knowledge correctly (left) and is more efficient than our previously developed Bayesian Optimization Structure Search method.



[1] B. Alldritt, P. Hapala, N. Oinonen, F. Urtev, O. Krejci, F. F. Canova, J. Kannala, F. Schulz, P. Liljeroth, A. S. Foster, Sci. Adv. 6, eaay6913 (2020)
[2] P. Mikkola, M. Todorović, J. Järvi, P. Rinke and S. Kaski, In Proceedings of the 37th International Conference on Machine Learning, ICML'20, pp. 4050-4058, 2020
[3] M. Todorović, M. U. Gutmann, J. Corander and P. Rinke, npj Comp. Mat. 5, 35 (2019)

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Finnish Center for Artificial Intelligence FCAI is a community of experts in 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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