CENTER FOR MOLECULAR MODELING

GHENT UNIVERSITY

Incremental Learning for ‘more challenging’ systems

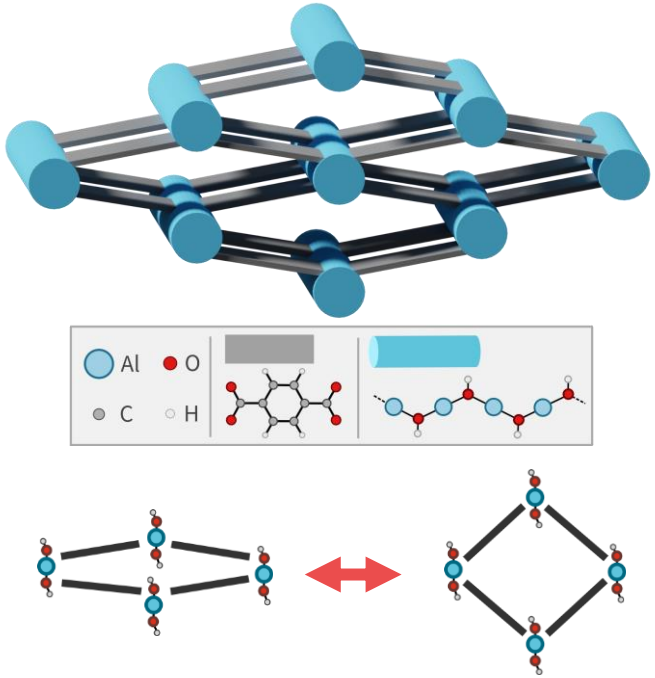
Sander Vandenhaute

advisor: Veronique Van Speybroeck

Research Foundation Flanders
Opening new horizons

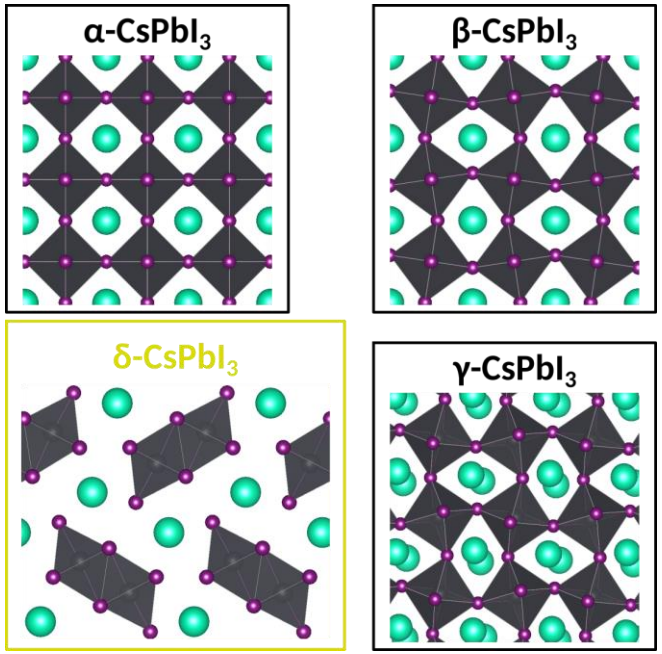
European Research Council

activated processes are everywhere



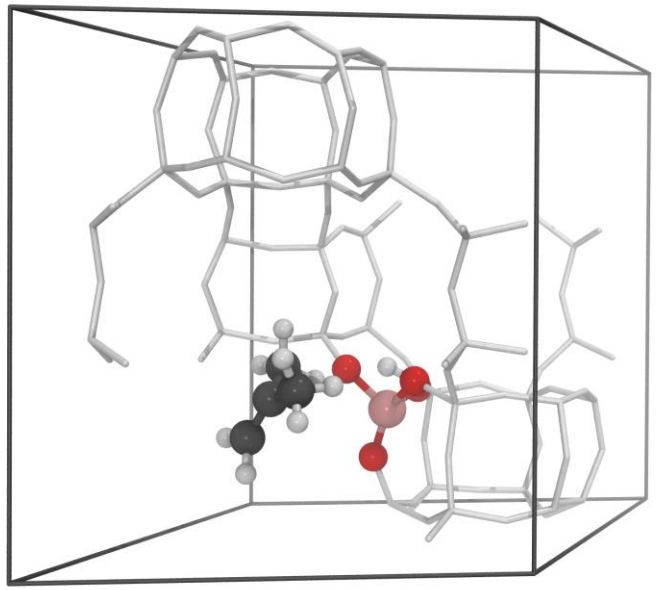
nanoporous materials

collective variable:
pore volume



perovskites

collective variable:
strain tensor

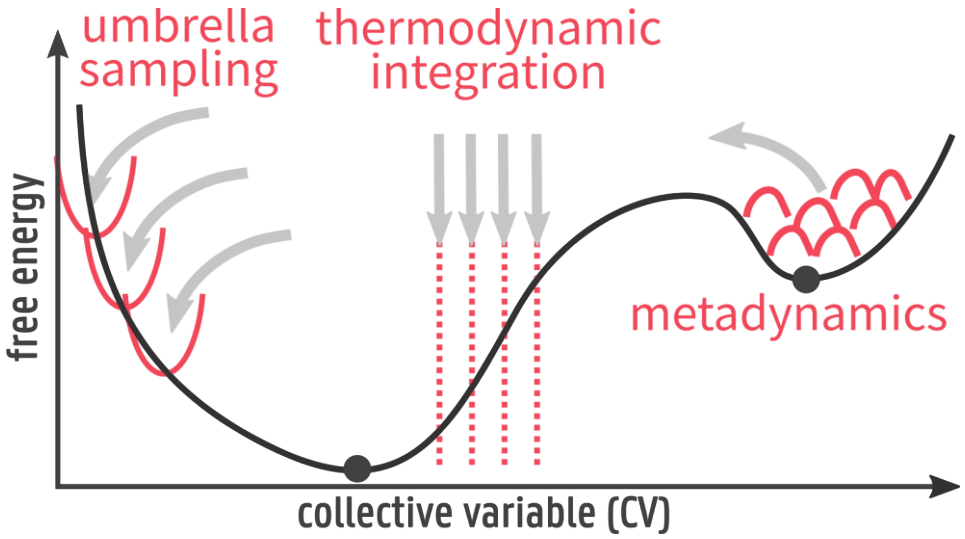


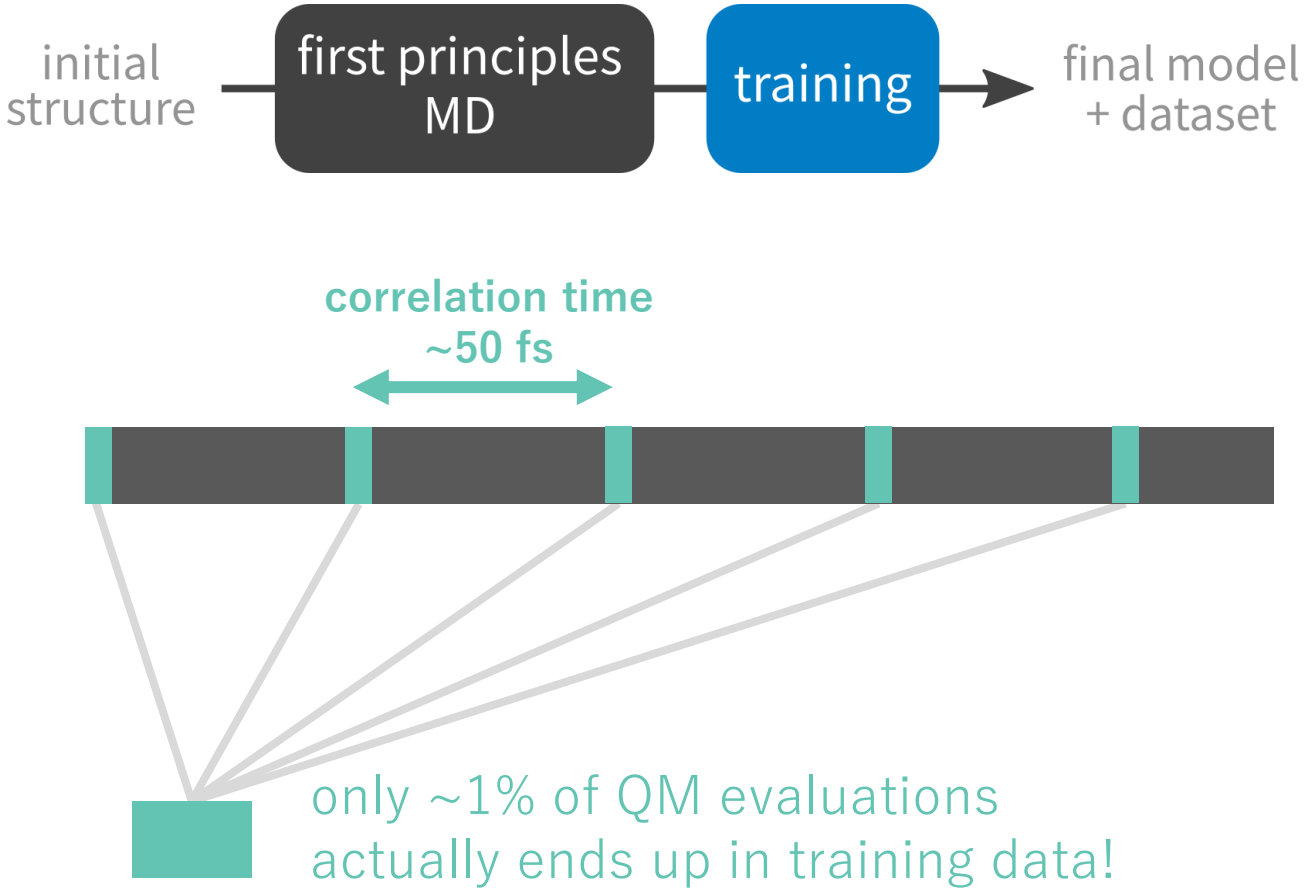
zeolite catalysis

collective variable:
coordination numbers

the key challenge: data generation!

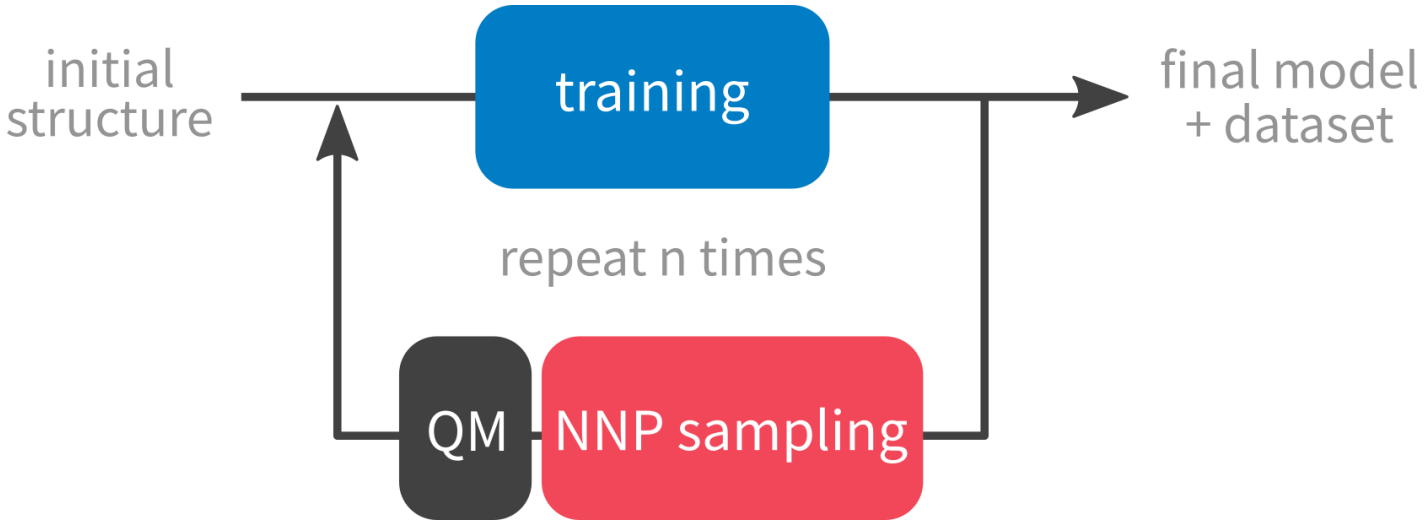
first principles MD is demonstrably inefficient

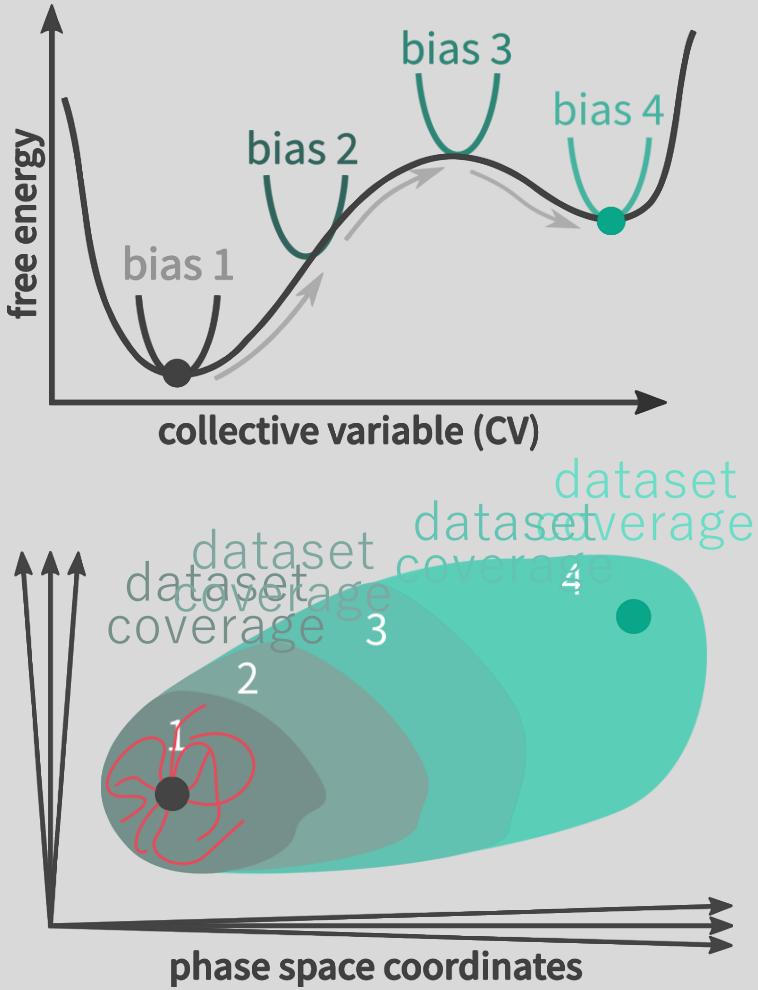




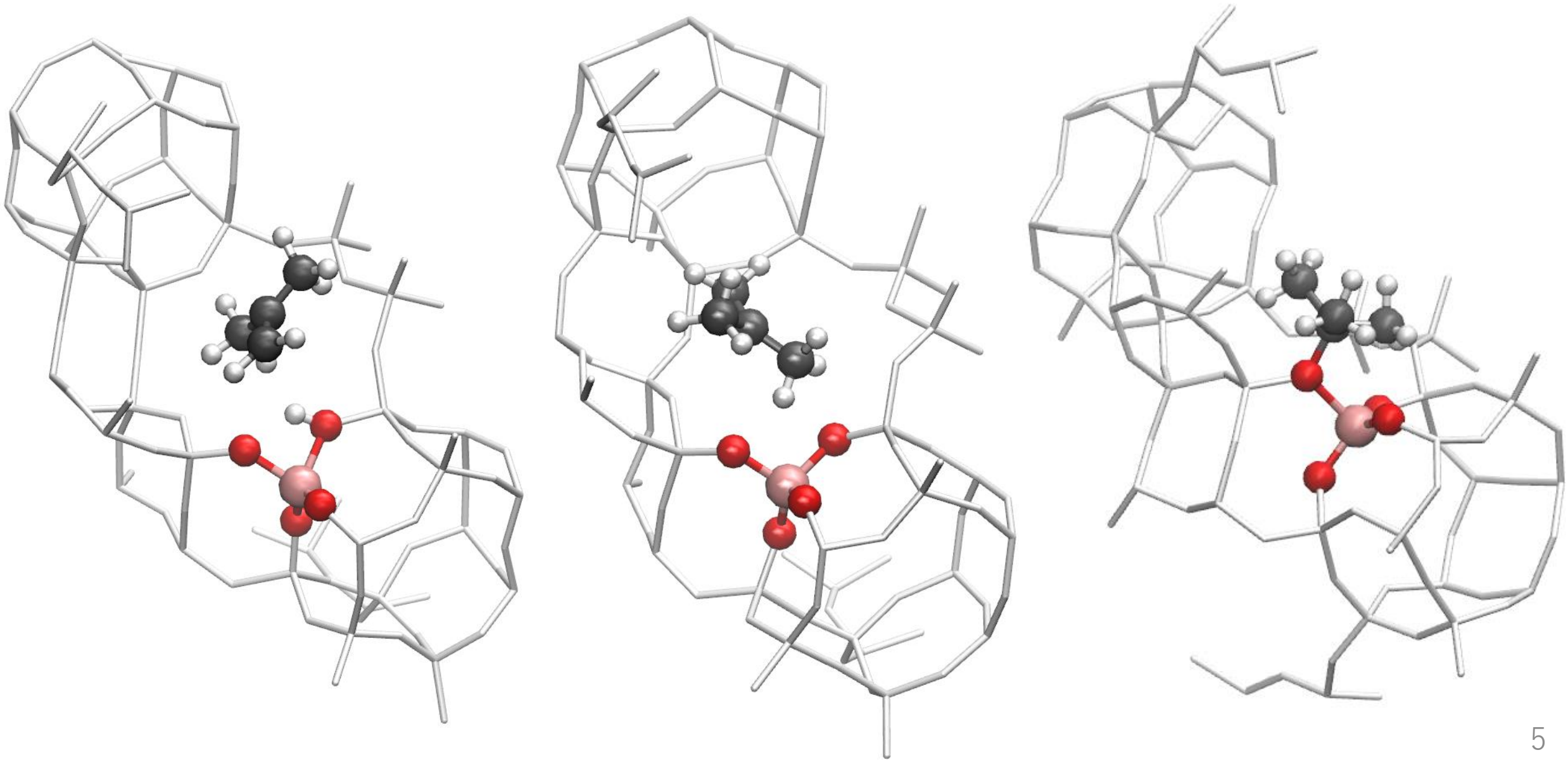
“incremental learning”

interleave training with short (multiple-walker) sampling

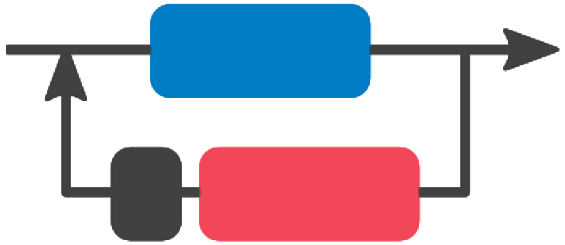


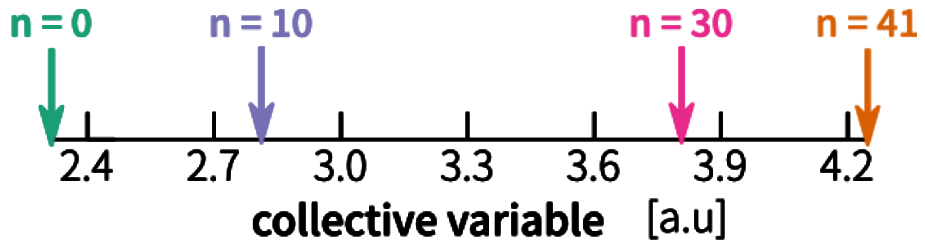


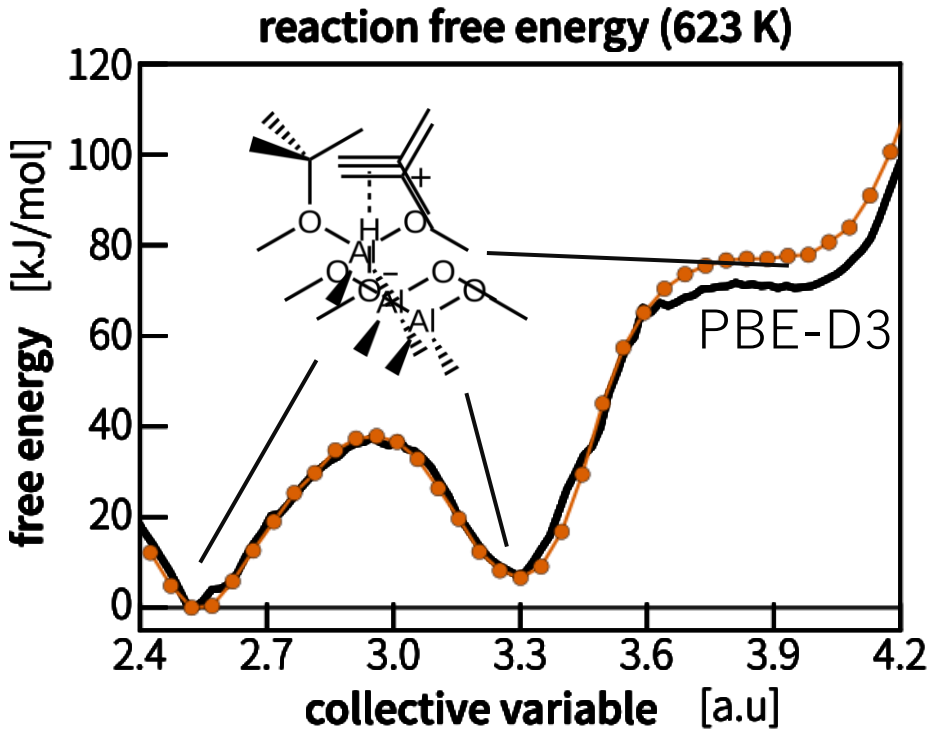
isobutene <> carbenium ion <> surface alkoxide

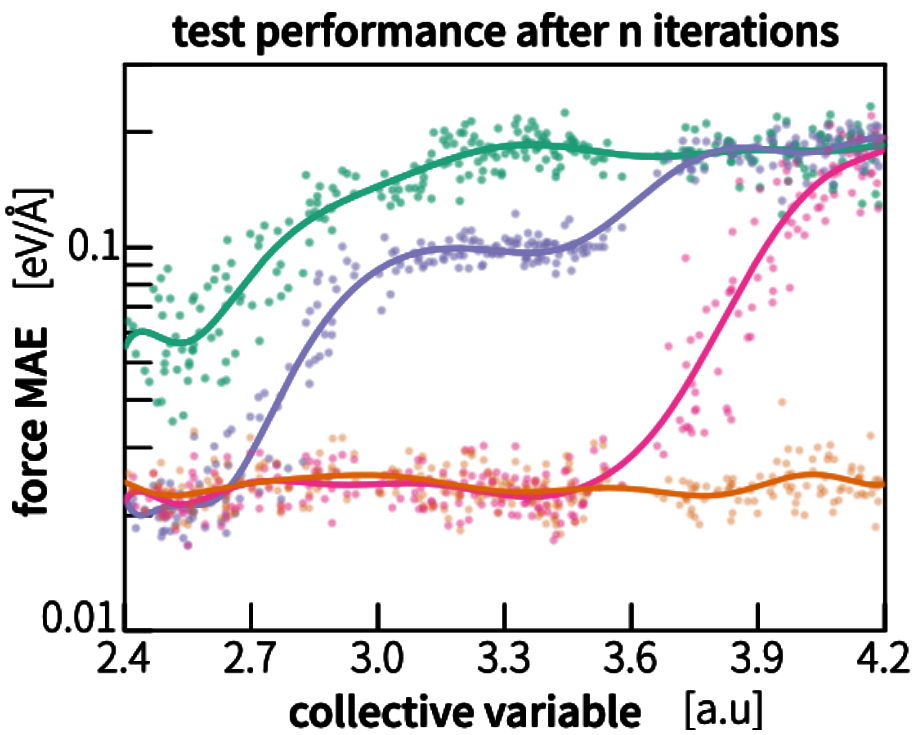


isobutene <> carbenium ion <> surface alkoxide

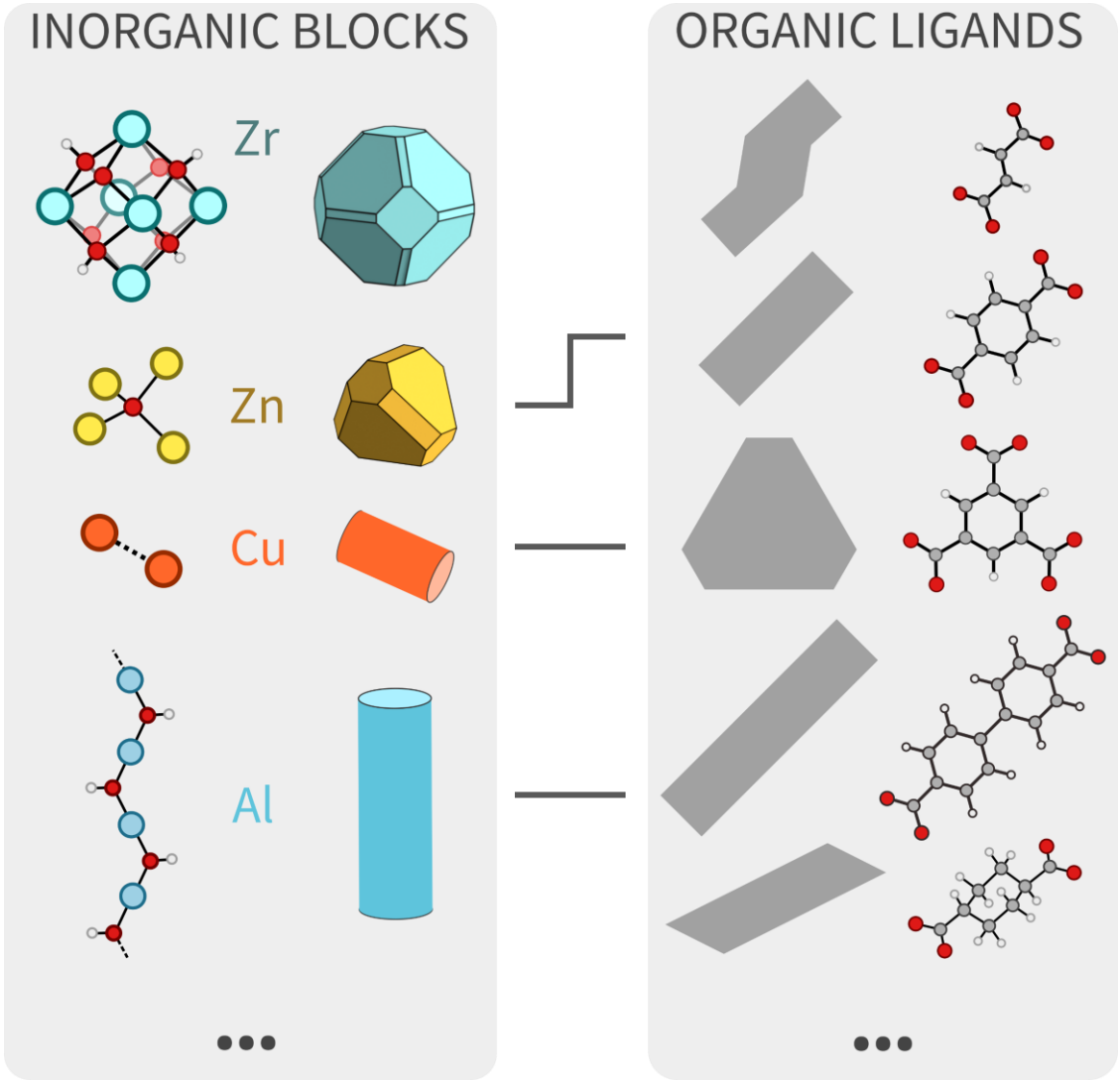


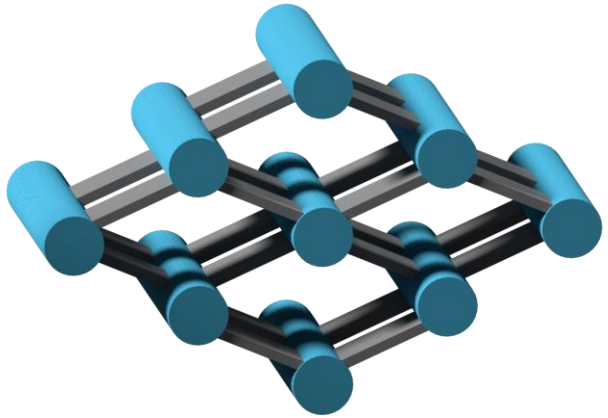


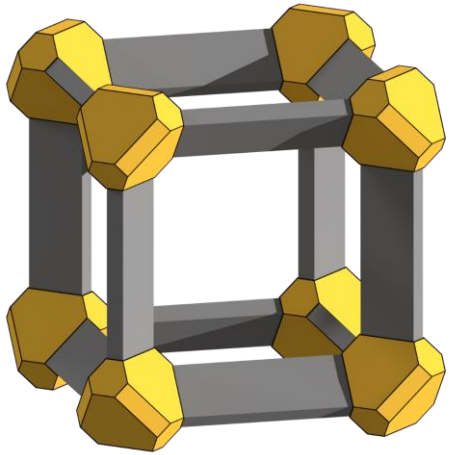


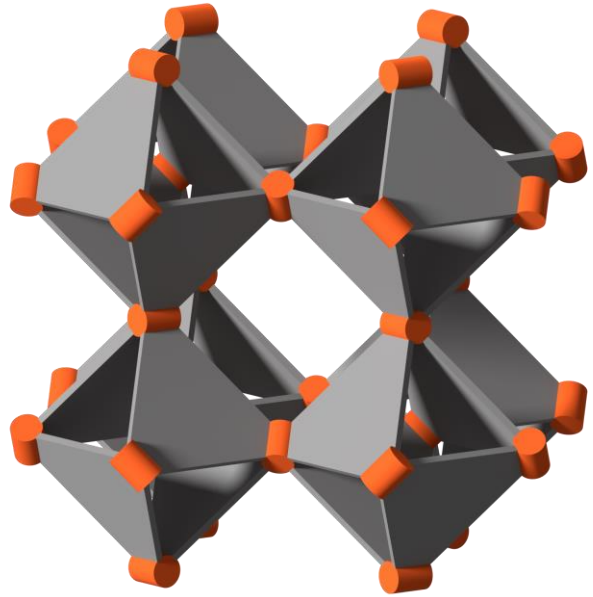


incremental learning for multiple materials?



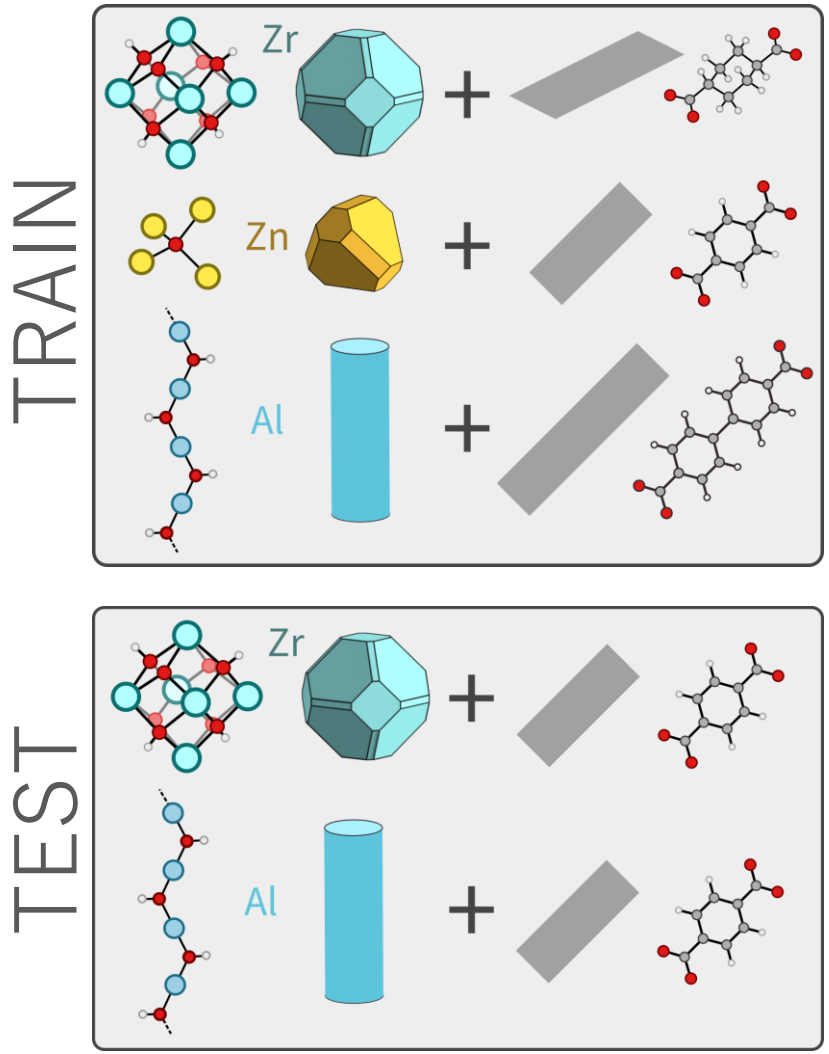


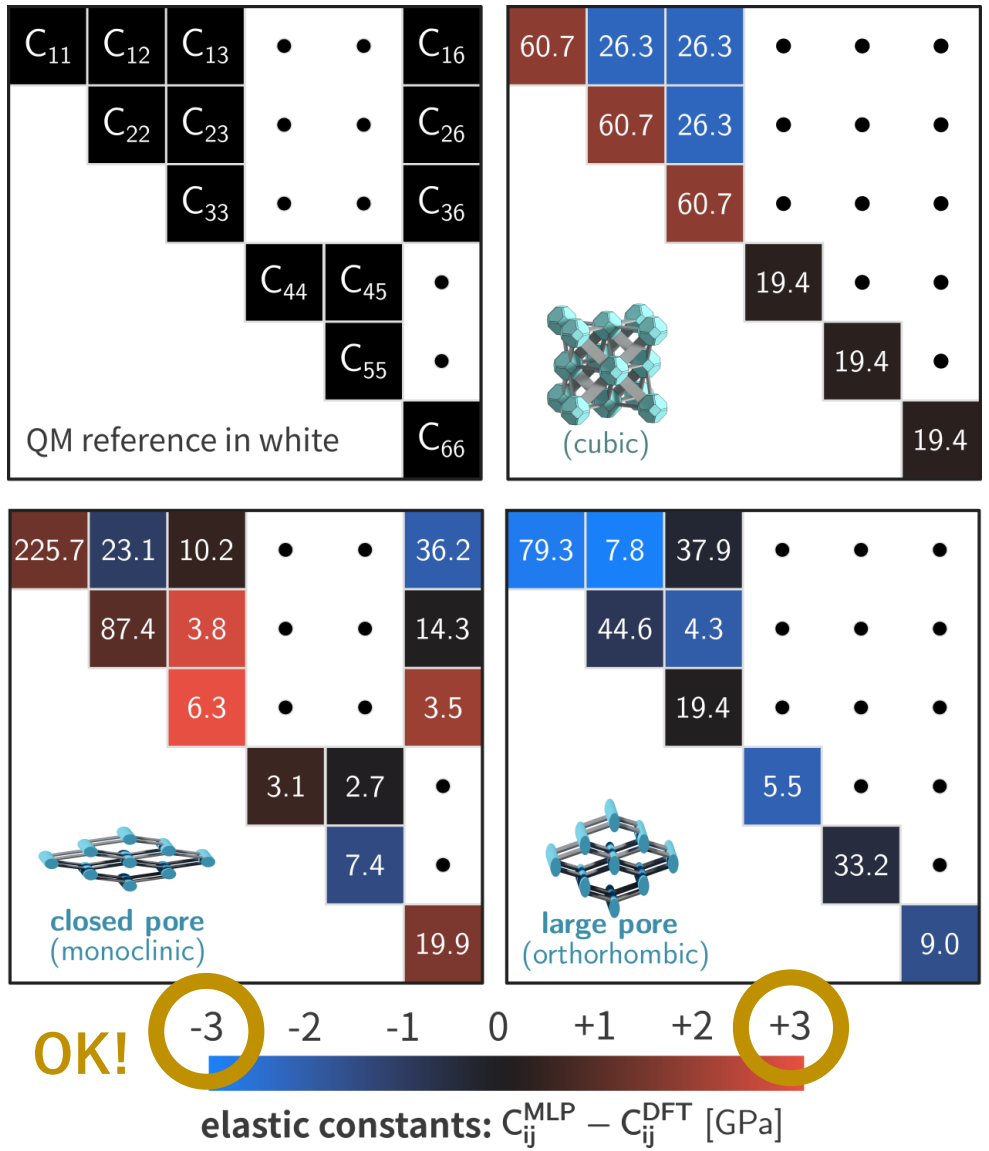




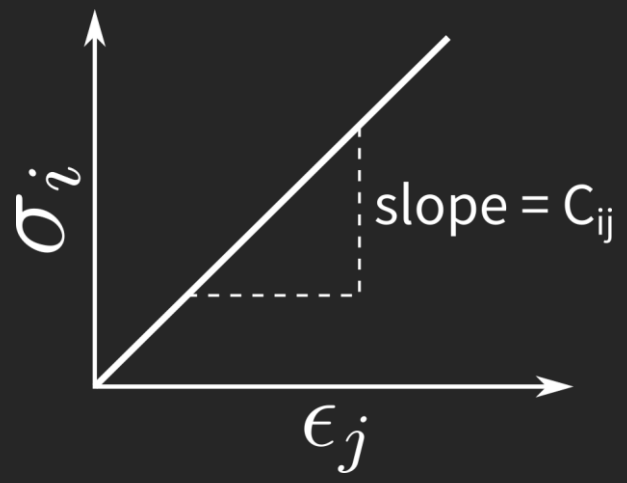
transferability towards ‘unseen’ combinations!

example: **mechanical properties**





… exploit automatic differentiation!

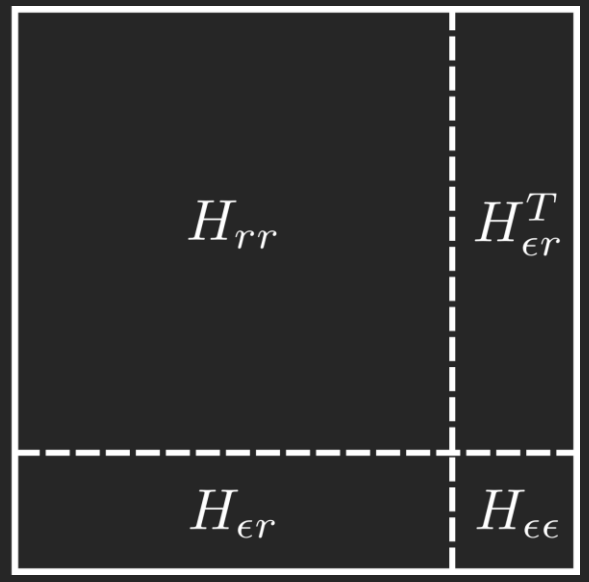


$$C_{ij} \sim \left(\frac{\partial^2 U}{\partial \epsilon_i \partial \epsilon_j} \right)_{\text{optimized positions}}$$

$$\vdots$$

$$C \sim H_{\epsilon\epsilon} - H_{\epsilon r} H_{rr}^{-1} H_{\epsilon r}^T$$

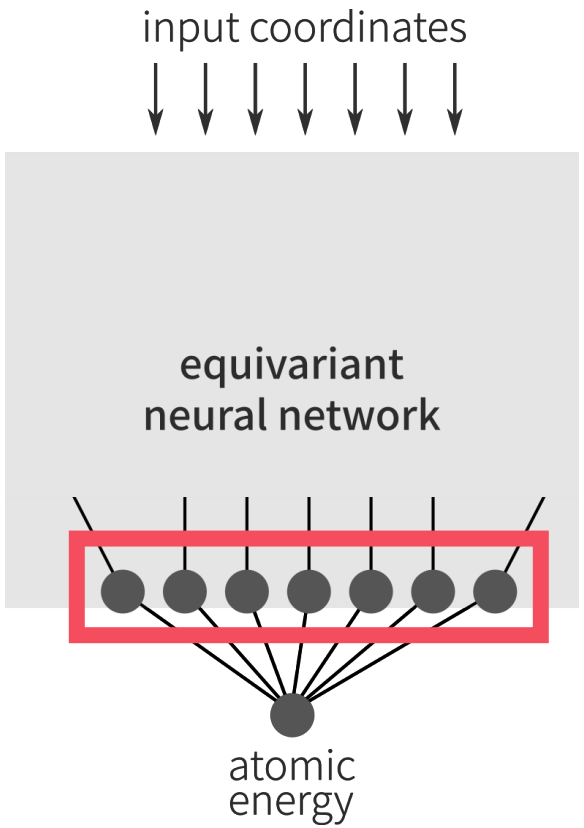
extended hessian:



achieves **double** precision!

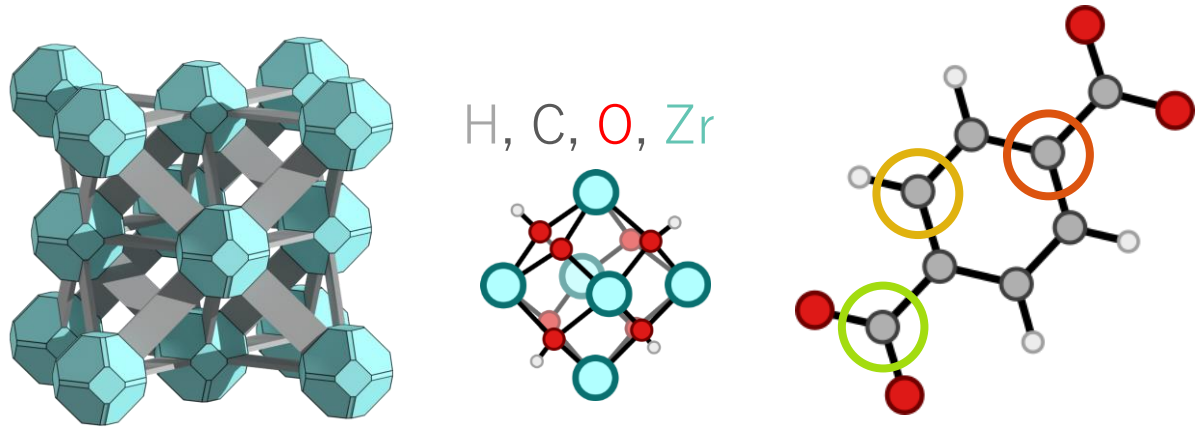
can we easily predict transferability?

analyze final output layer!

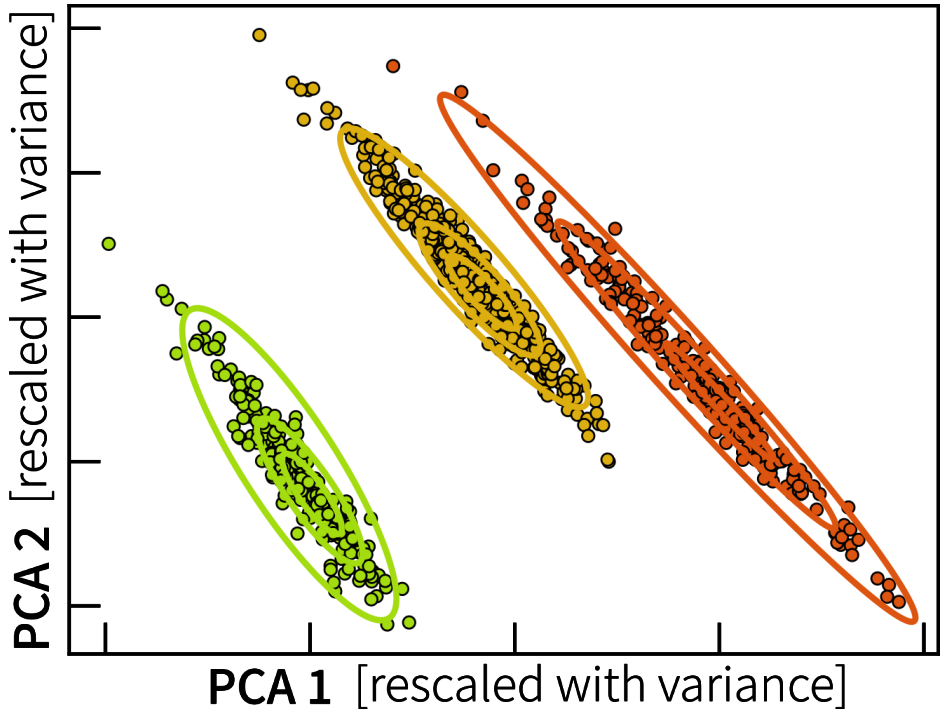


extract for C

apply PCA



P(environment | data) !



contains all the information necessary to predict the atomic energy, in a low-dimensional space! (d~10)

thank you!

Veronique Van Speybroeck

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Sven M. J. Rogge
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