

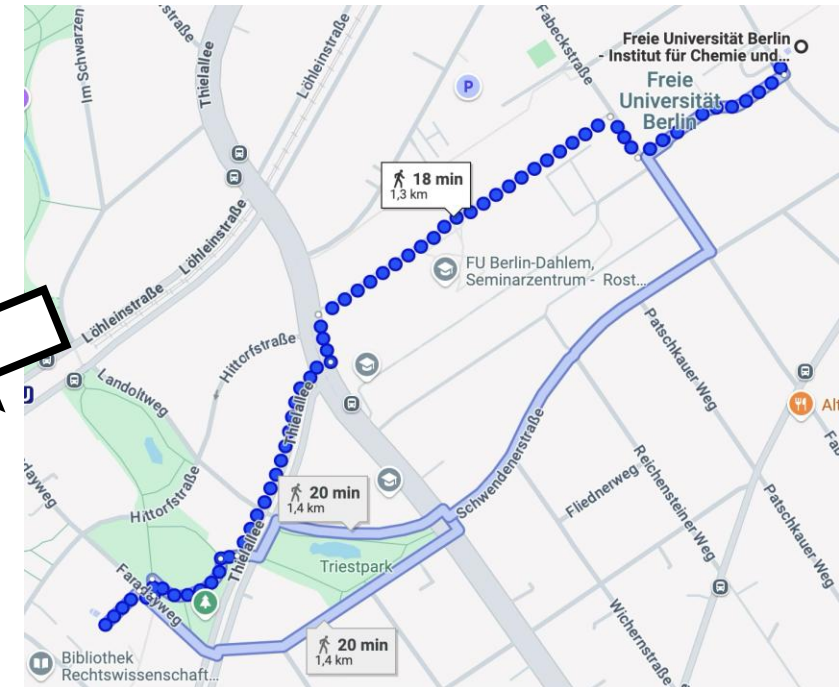


Research Topics at the Theory Department of the Fritz Haber Institute

Opportunities for Internships, BSc & MSc Theses

Research & Drinks – 12.11.2025

The Fritz Haber Institute



- ~ 500 Scientists
- 5 Departments
- Rich **history** of science

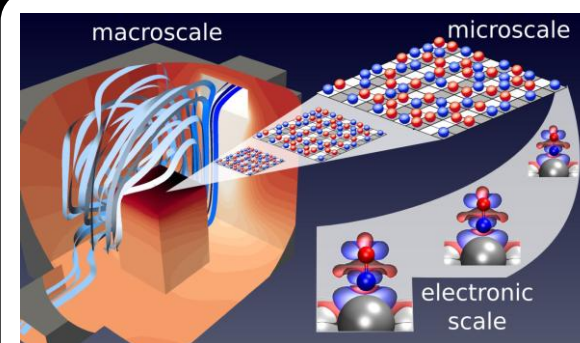
Theory Department of the Fritz Haber Institute



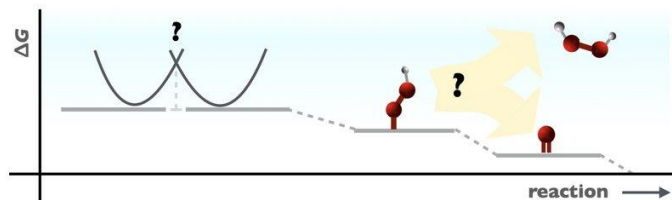
Light Matter Interactions
in Energy Materials



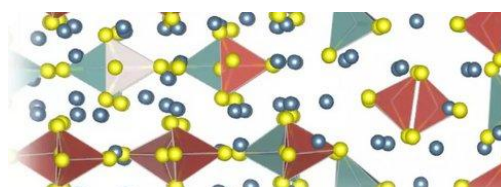
Computational
Mechanochemistry



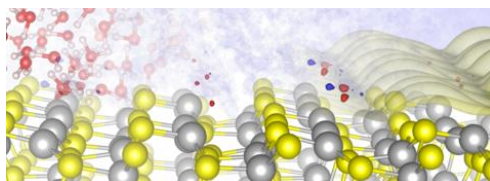
Multiscale Modeling from
the Electron to the Reactor



Selectivity in catalysis



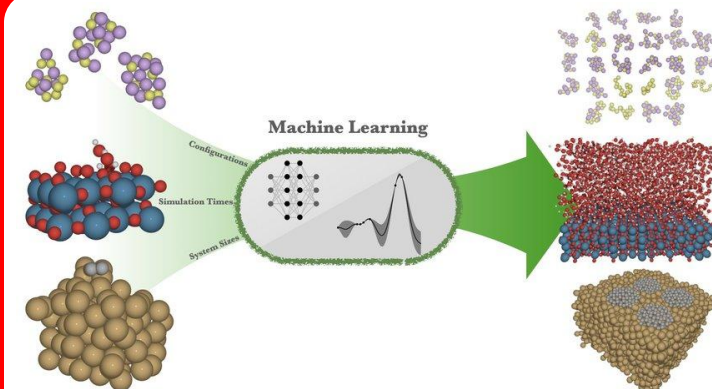
Operando evolution of battery materials
and functional solid-solid interfaces



First-principles Modeling of Solid-Liquid
Interfaces and Electrocatalysis



Theory of Heat and Charge
Transport at Interfaces



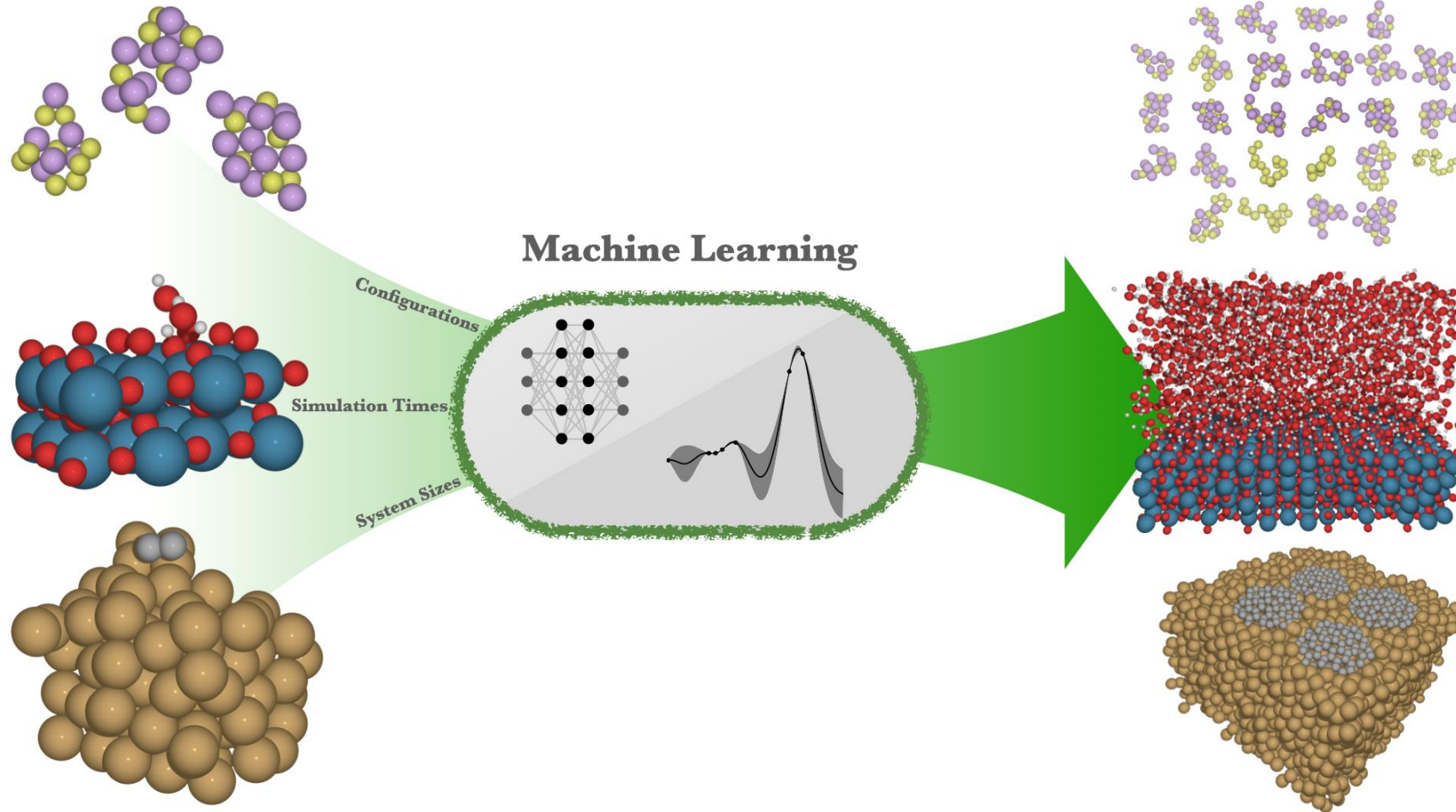
Interatomic machine learning
potentials for energy materials



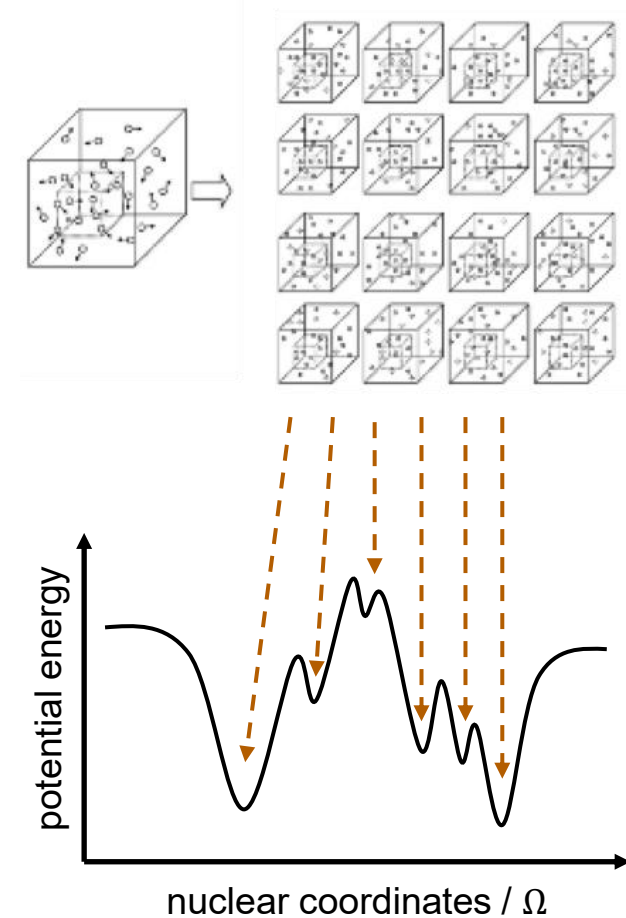
Complex (surface) chemistry: Scaling-up & Sampling

Interfacial & conversion chemistry ...

... requires sampling

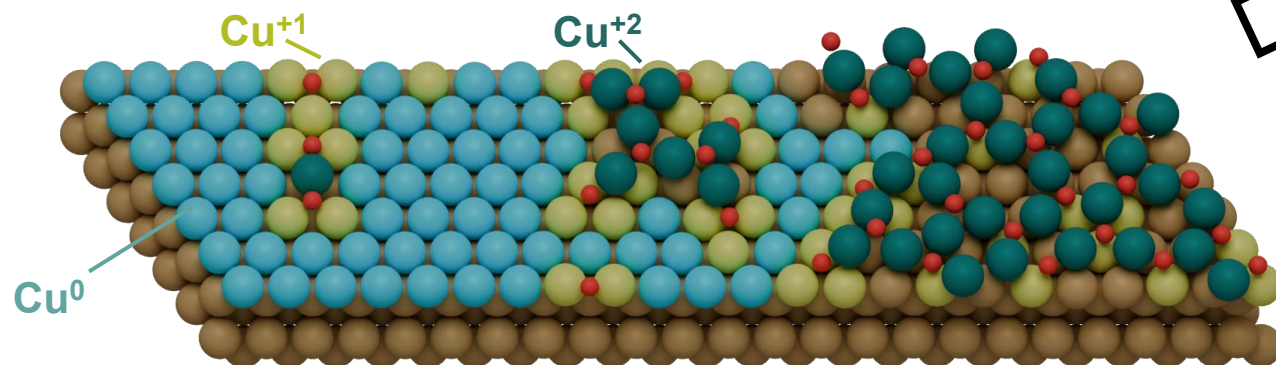


Statistical Thermodynamics

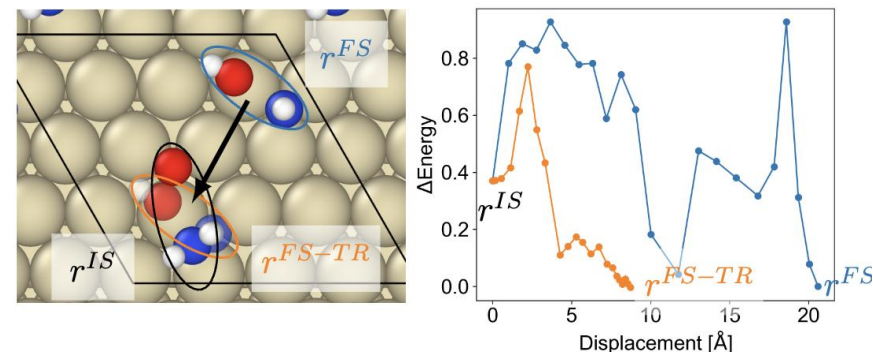


Topics: Catalyst surfaces

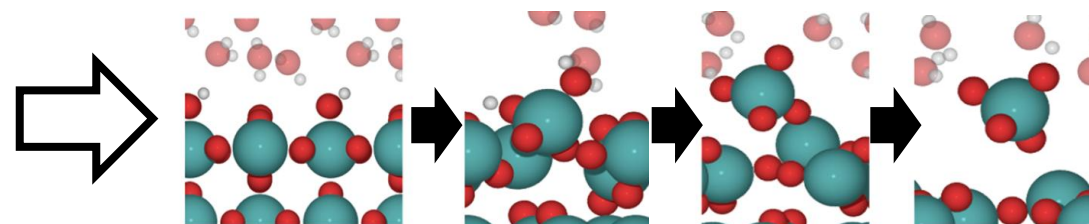
Surface evolution



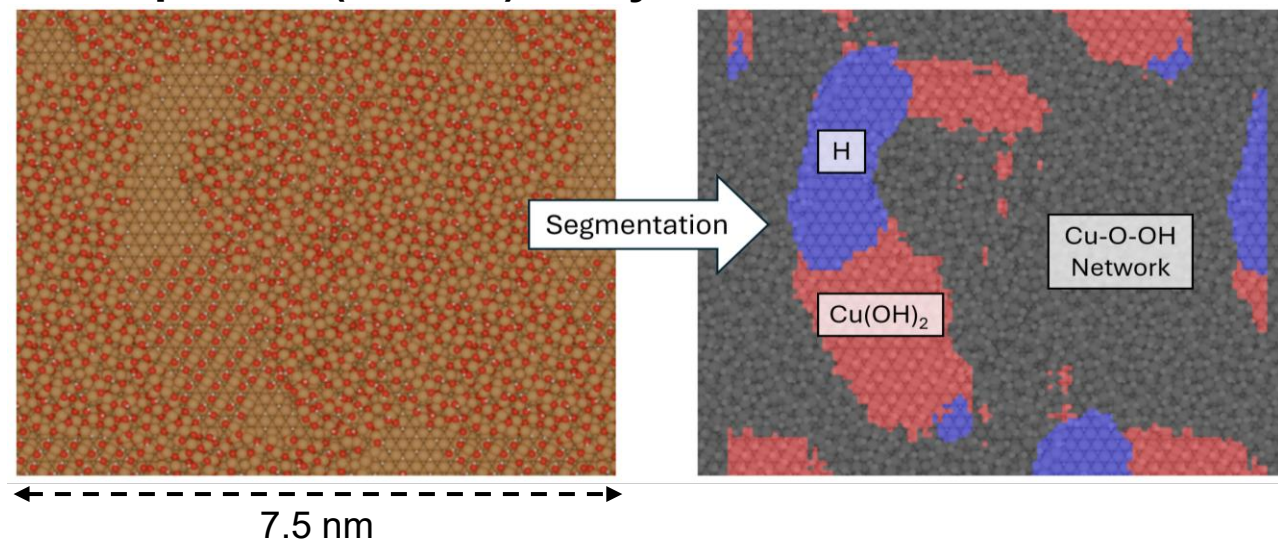
activity & selectivity



degradation

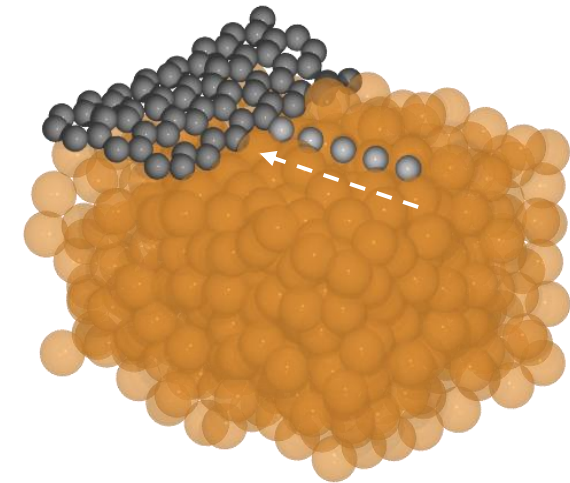
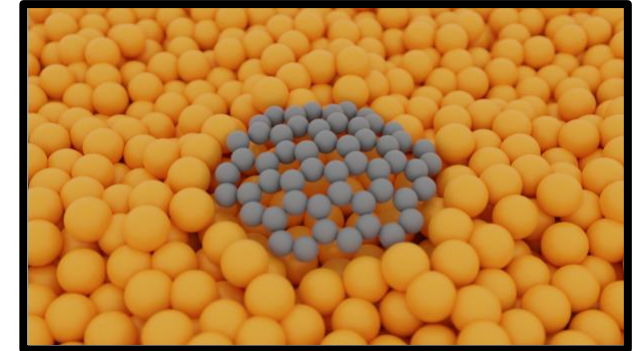
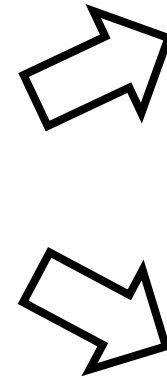
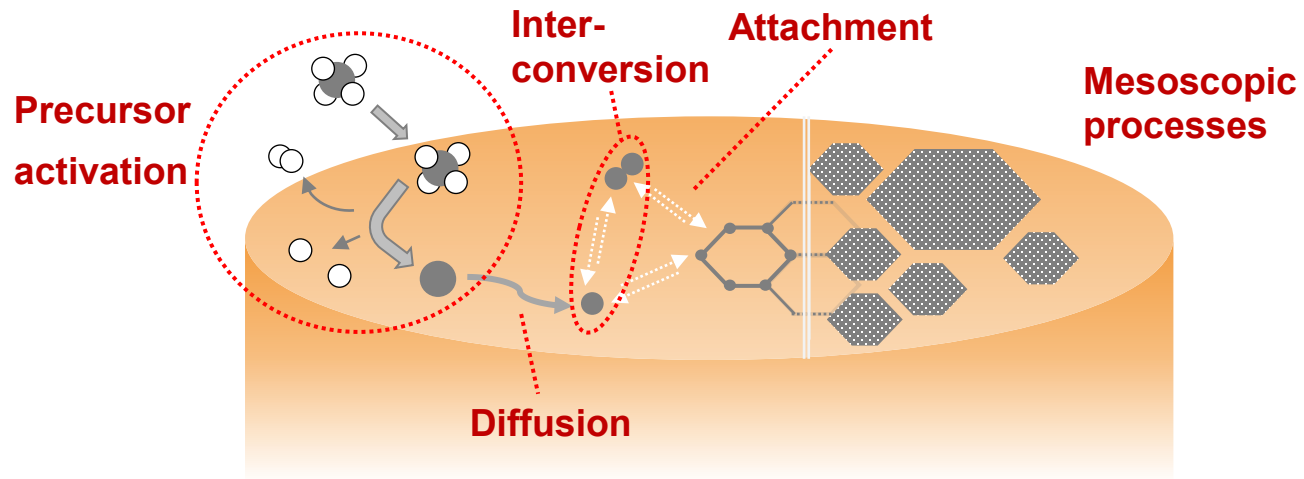


Example: Cu (electro)catalyst





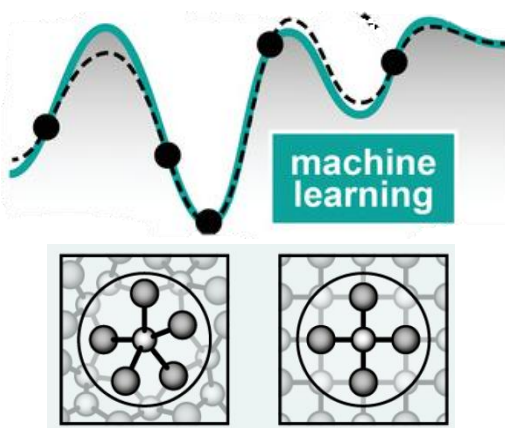
Topics: CVD of 2D-Materials on liquid metal catalysts



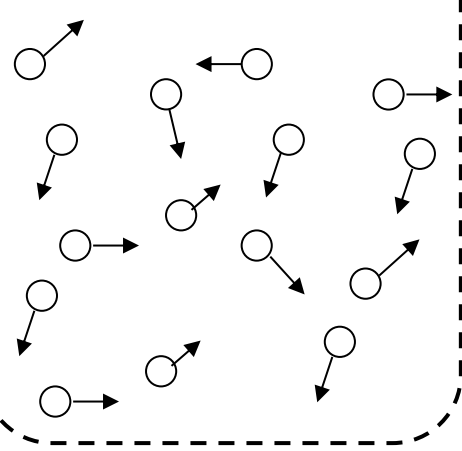


Methods

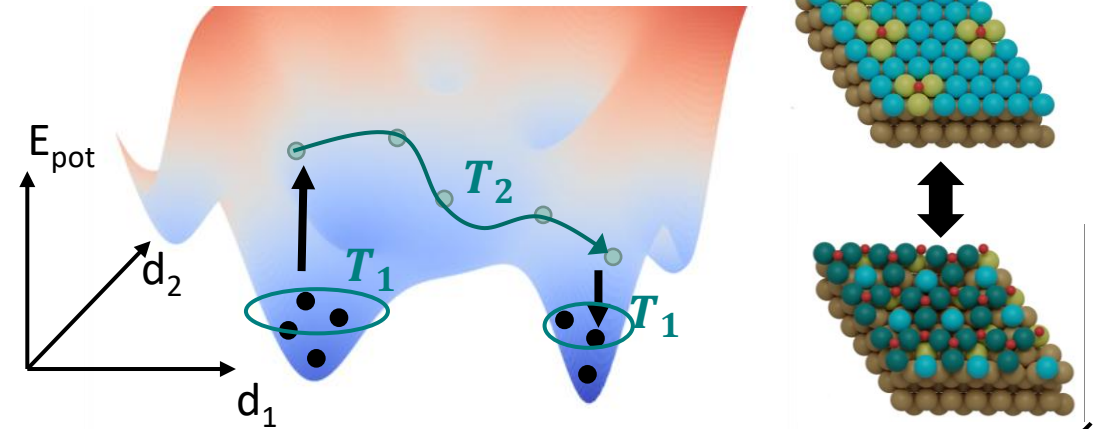
ML Interatomic Potentials



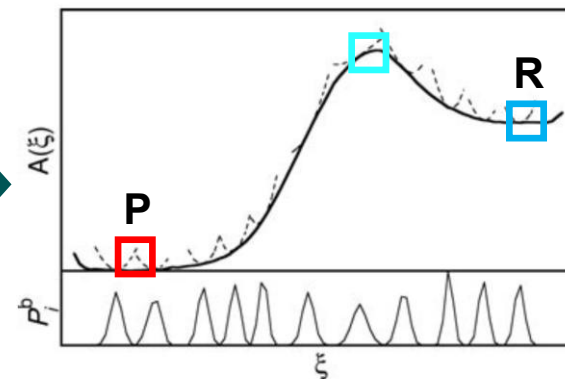
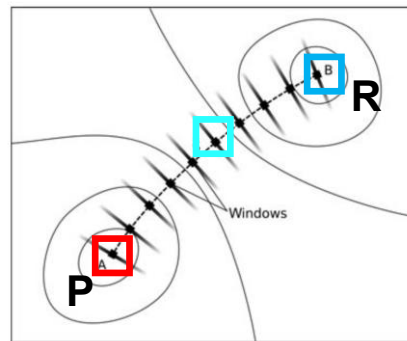
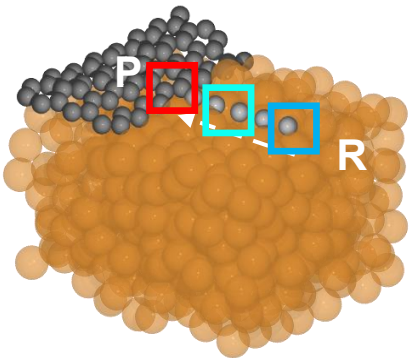
Molecular Dynamics



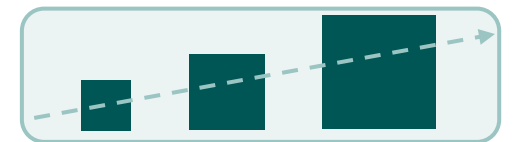
Accelerated sampling



Enhanced sampling



Multiscale modelling



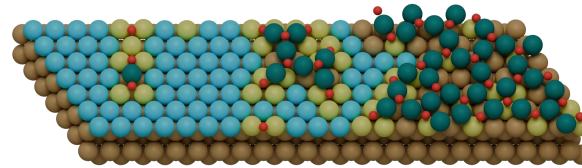
e.g. microkinetic models



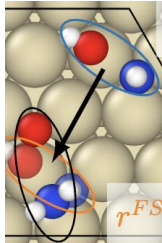
Summary

Machine Learning Interatomic Potentials for Energy Materials

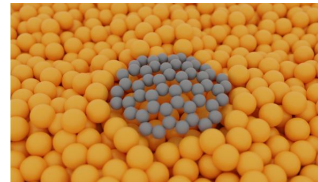
➤ Catalytic surface evolution



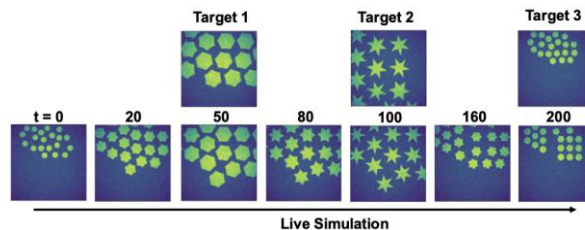
➤ & reactivity



➤ CVD film growth on liquid metals



➤ (AI agents and more)



Thank you for your
attention

Interested? ➡ heenen@fhi.mpg.de