



MATTER

Simulating electrostatic forces under electric fields using machine learning

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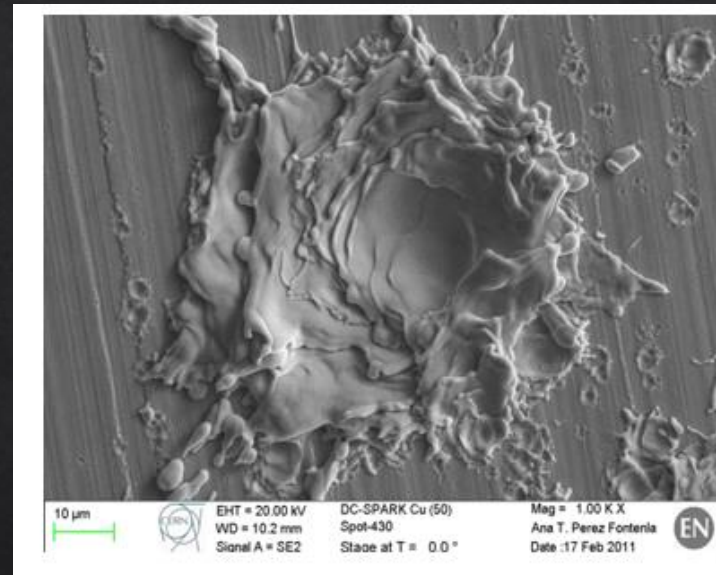


Overview

- Introduction
- DFT
- Machine Learning
- Conclusion
- Outlook

Introduction

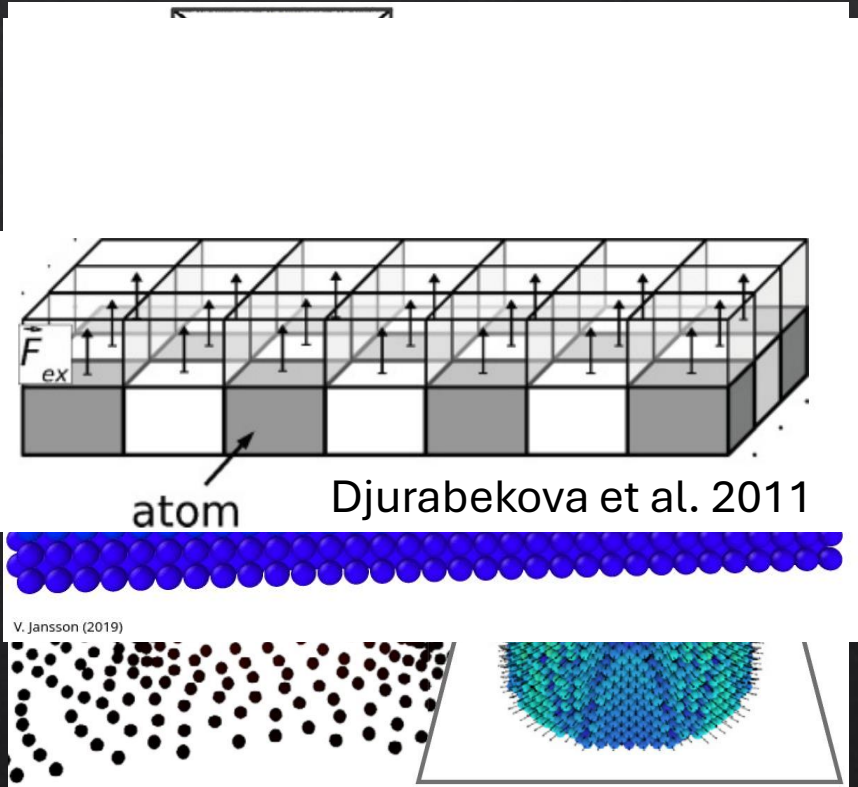
Problem: Formation of field-enhancing tips on metals



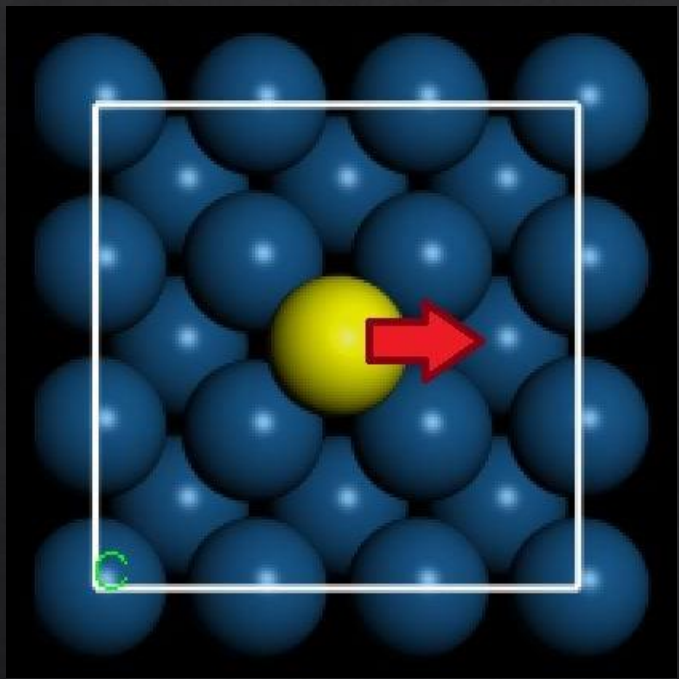
Goal: Understanding the underlying mechanism

Mechanisms

Maxwell stress



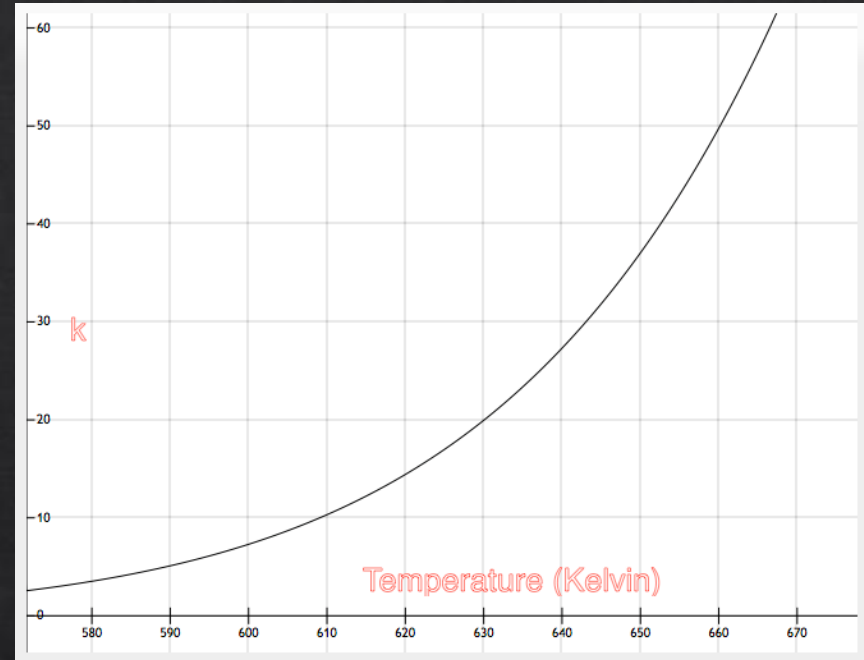
Surface diffusion



Diffusion is temperature dependent

Diffusion coefficient:

$$D = D_0 \exp\left(-\frac{E}{kT}\right)$$



Temperature → Molecular Dynamics (MD)

How to simulate surface diffusion in MD?

We need **forces** for the molecular dynamics simulation.

Forces are derivatives of **potential**: $F_x = -\frac{\partial U}{\partial x}$

Potential is a function of atomic positions and electric field (E):

$$U = U(x, E)$$

From the Taylor series: $U = U_0 - \frac{\partial U}{\partial E} E - \frac{1}{2} \frac{\partial^2 U}{\partial E^2} E^2$

μ : Dipole moment

$$U = U_0 - \mu E - \frac{1}{2} \alpha E^2$$

α : Polarizability



What parameter do we need?

To predict forces (F_x) we need:

$-\frac{\partial U_0}{\partial x}$: Interatomic forces	μ : dipole moment α : polarizability	E : electric field
Molecular dynamics	Machine learning from DFT	Finite Element Method

$$U = U_0 - \mu E - \frac{1}{2} \alpha E^2$$

$$F_x = -\frac{\partial U}{\partial x} = -\frac{\partial U_0}{\partial x} + \frac{\partial \mu}{\partial x} E + \frac{1}{2} \frac{\partial \alpha}{\partial x} E^2 + (\mu + \alpha E) \frac{\partial E}{\partial x}$$

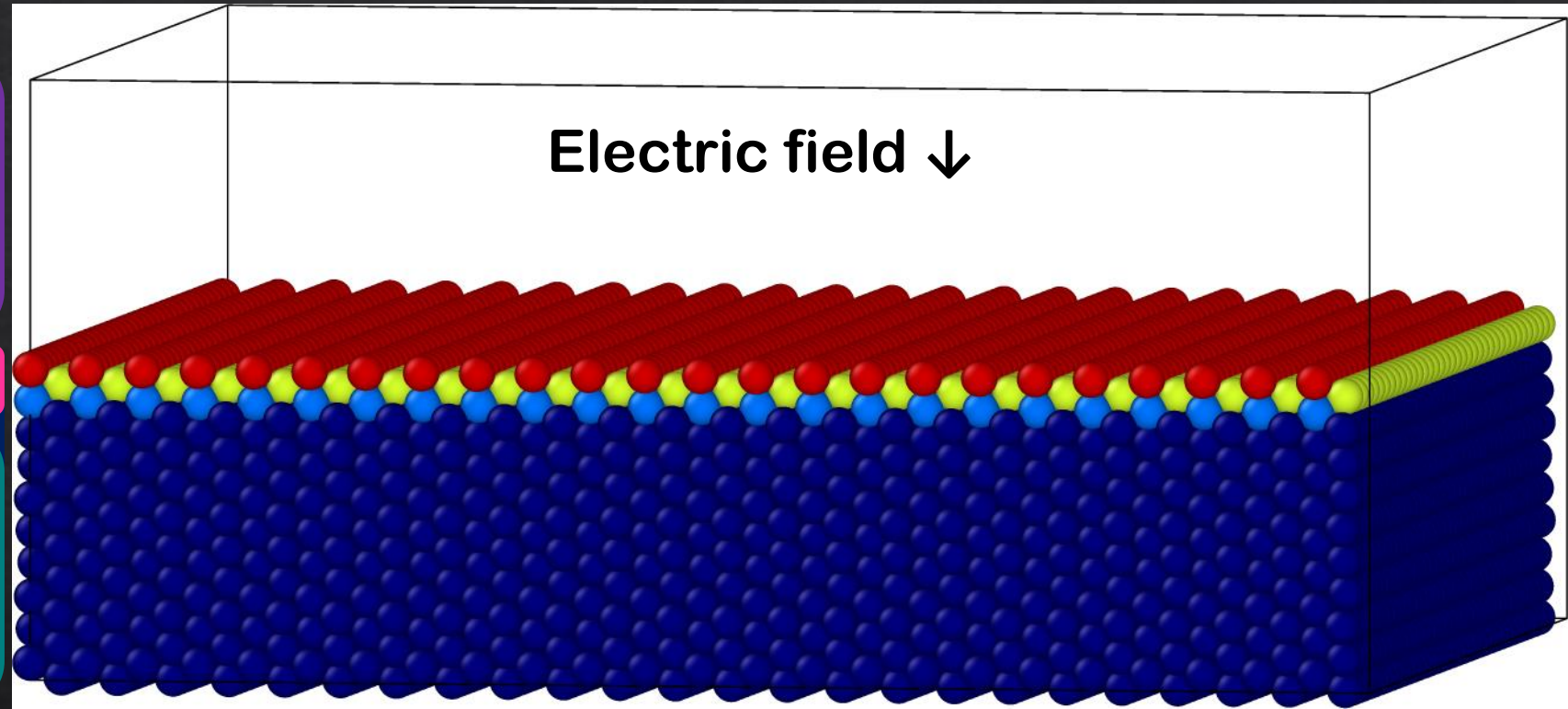
Multiscale Multiphysics Simulation

Electric field
from Finite
Element Method

Machine Learning

Newtonian
molecular
dynamics
(cheap)

Learned
from DFT





Overall process

Produce
accurate DFT
data

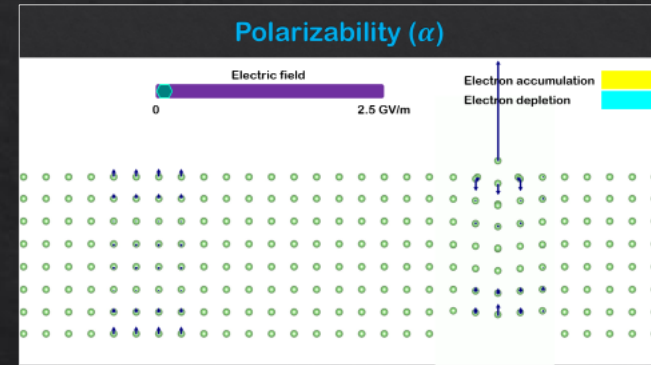
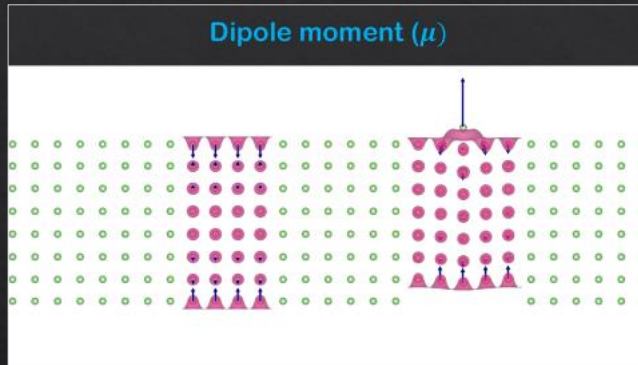
Train a Machine
Learning model
to predict forces

Hybrid
Molecular
Dynamics

Density Functional Theory (DFT)

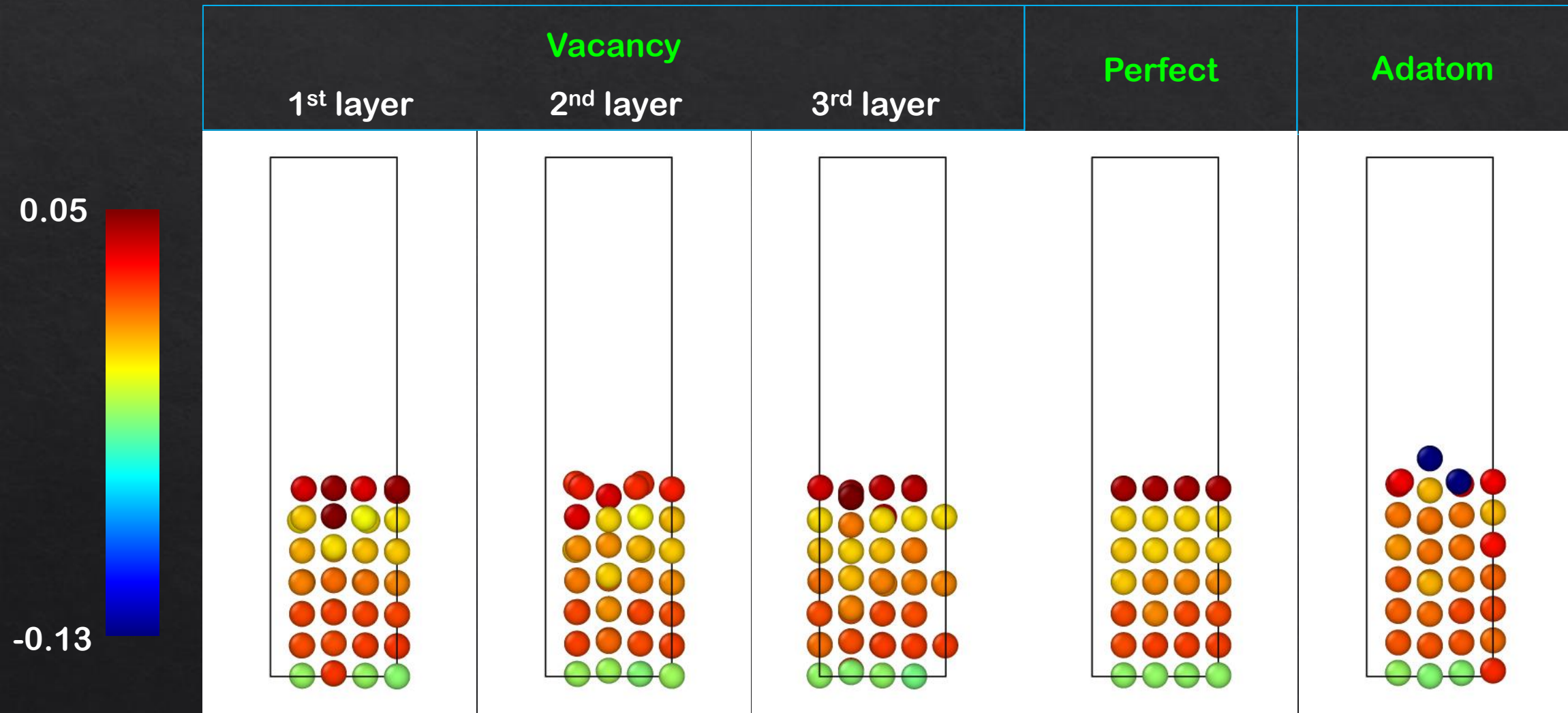
Dipole moment (μ) and polarizability (α)

$$U = U_0 - \mu E - \frac{1}{2} \alpha E^2$$



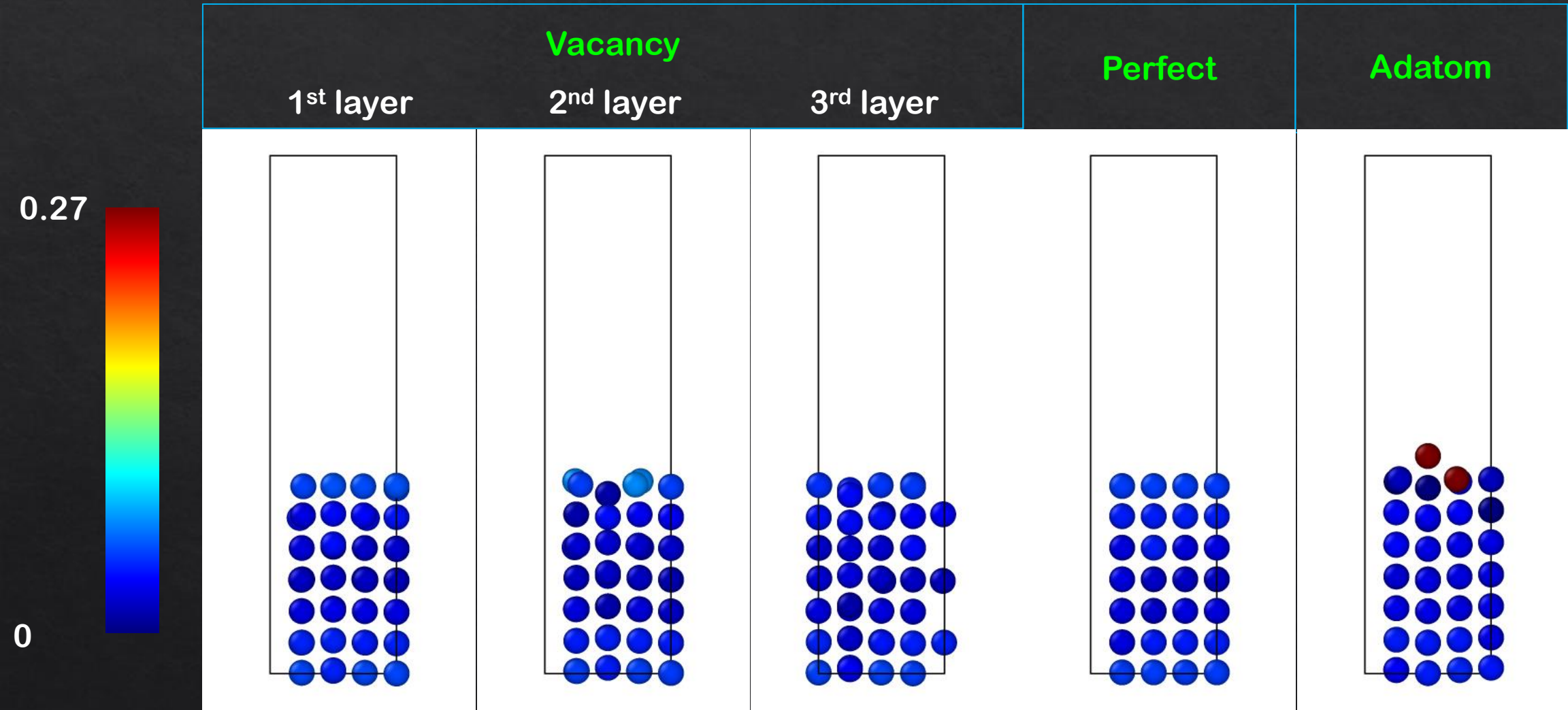
Local dipole

depends on the **local atomic environment**



Local polarizability

depends on the **local atomic environment**

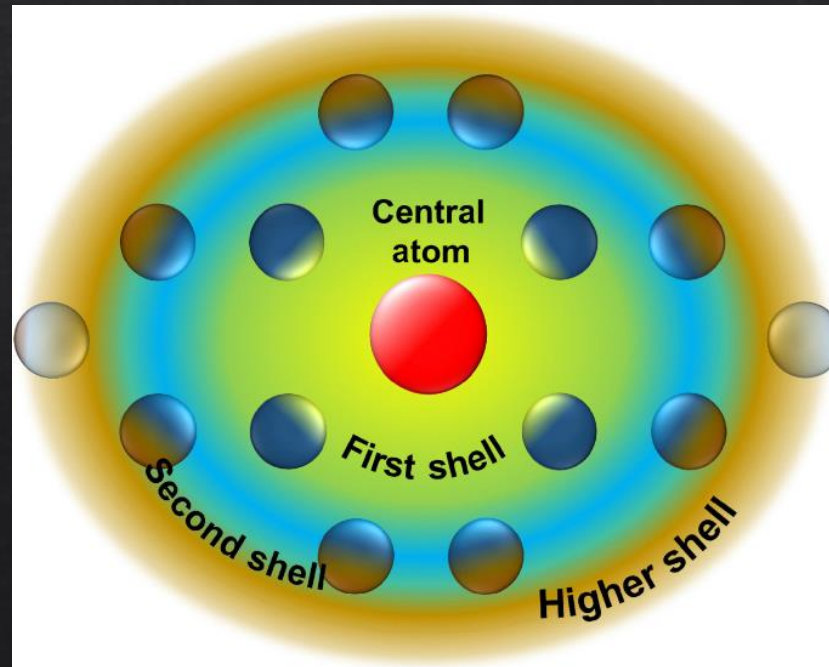


Machine Learning



Local Atomic Environment (LAE)

How to describe atoms to machines?





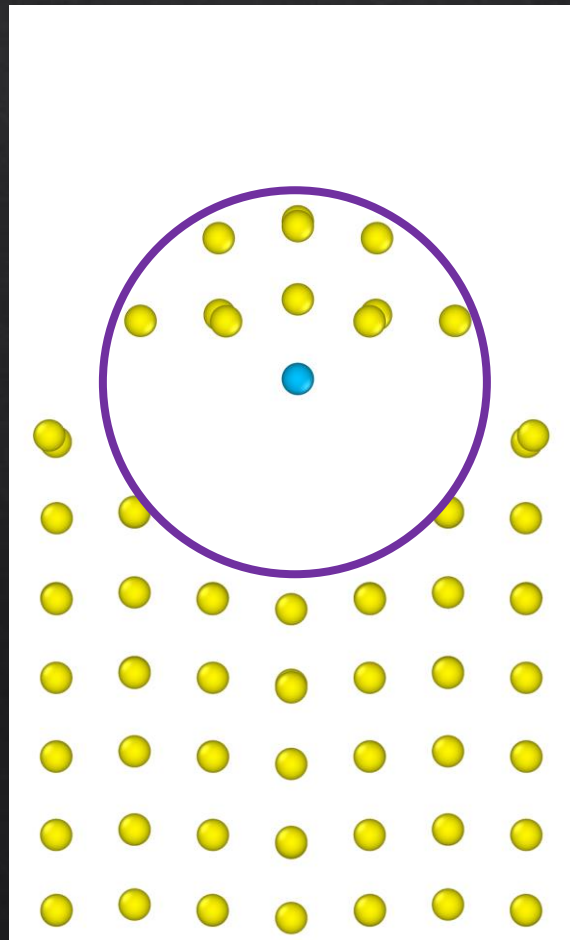
Local Atomic Environment

Dipole moment and polarizability depend on **LAE**

Potential Energy: 1.72 eV

Dipole moment: -0.13 e.Å

Polarizability: 0.27 Å³





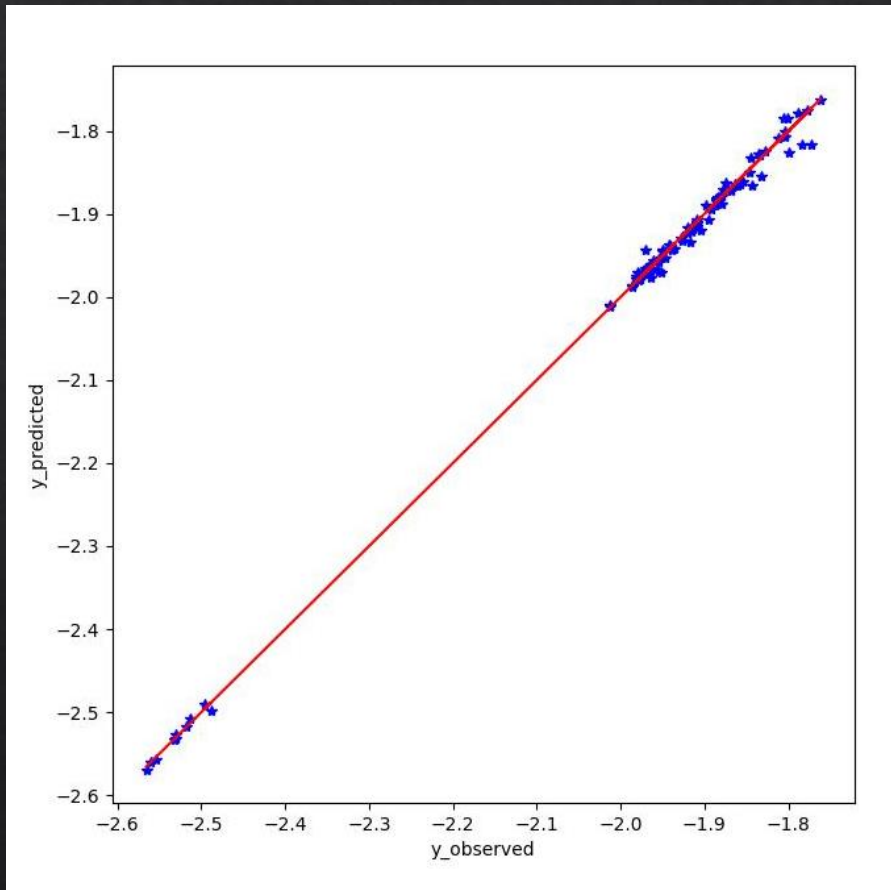
Descriptors: SOAP

Smooth Overlap of Atomic Positions

Invariance:

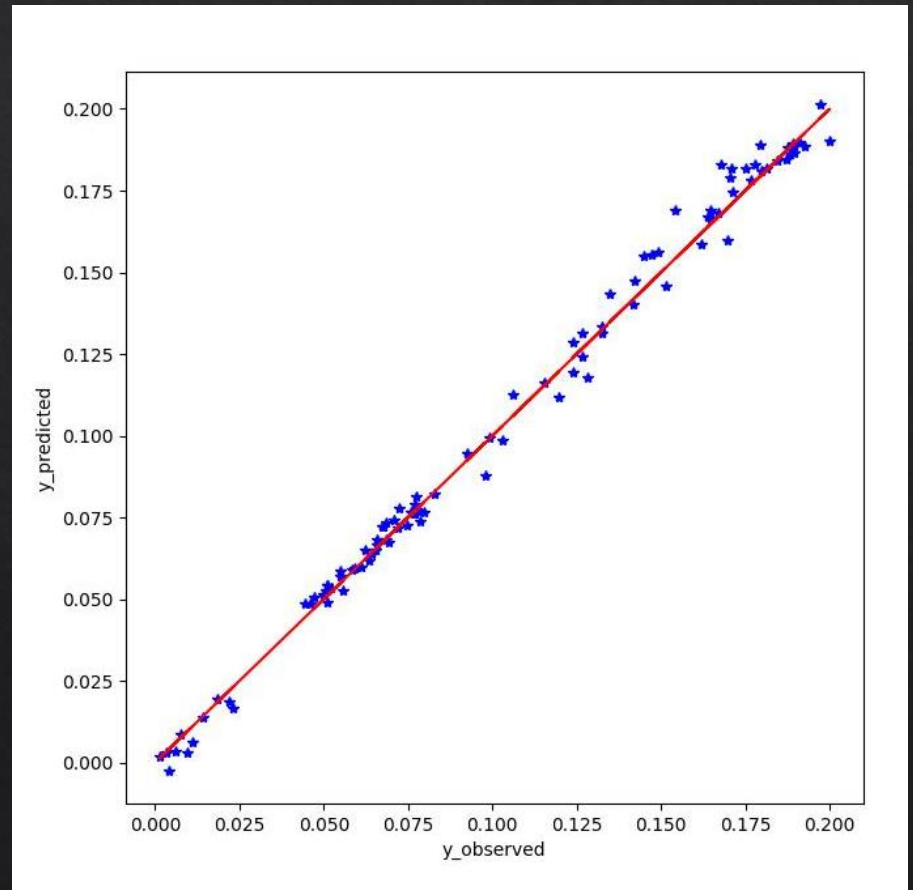
- ✓ Permutation
- ✓ Translation
- ✓ Rotation

RMSE: 0.01



Energy

RMSE: 0.005



Polarizability

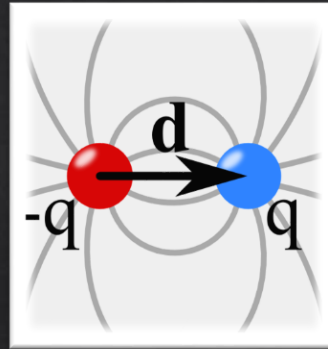
SOAP

Smooth Overlap of Atomic Positions

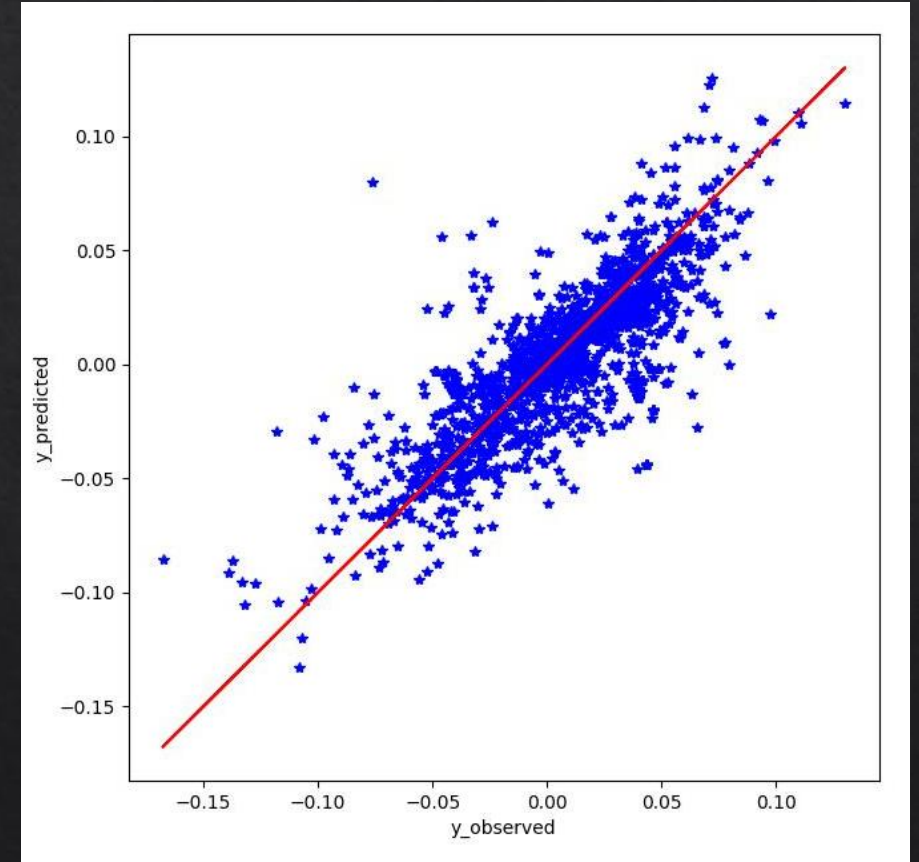
Invariance:

- ✓ Permutation
- ✓ Translation
- ✓ Rotation

SOAP doesn't know about **rotations**



RMSE: 0.024



Dipole moment



D-SOAP

Directional SOAP

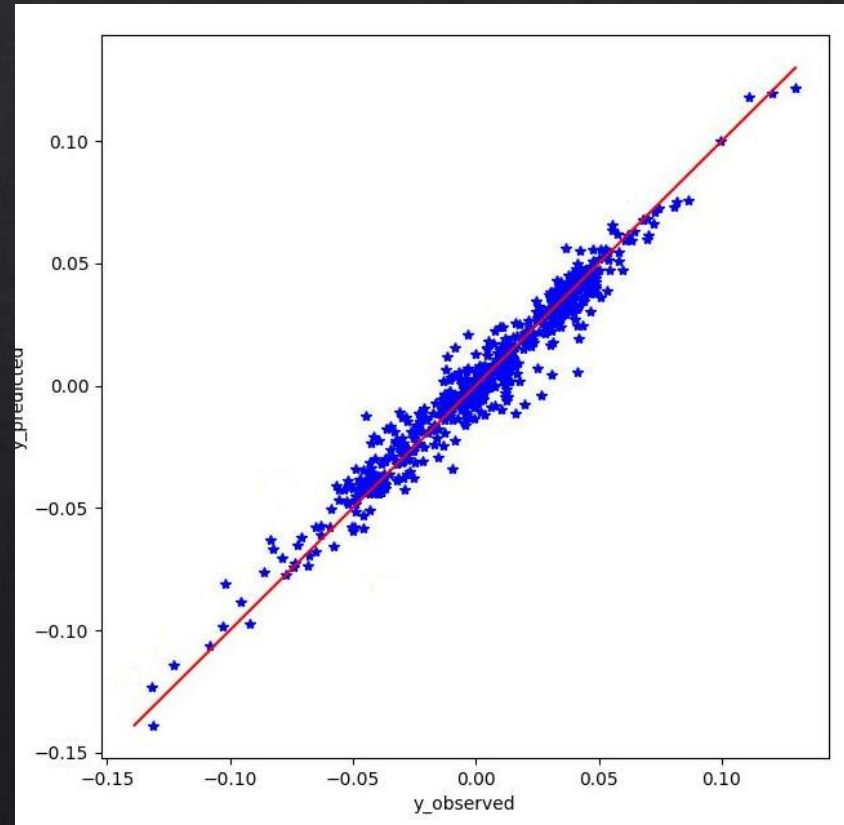
RMSE: 0.008

Invariance:

- ✓ Permutation
- ✓ Translation

Equivariance:

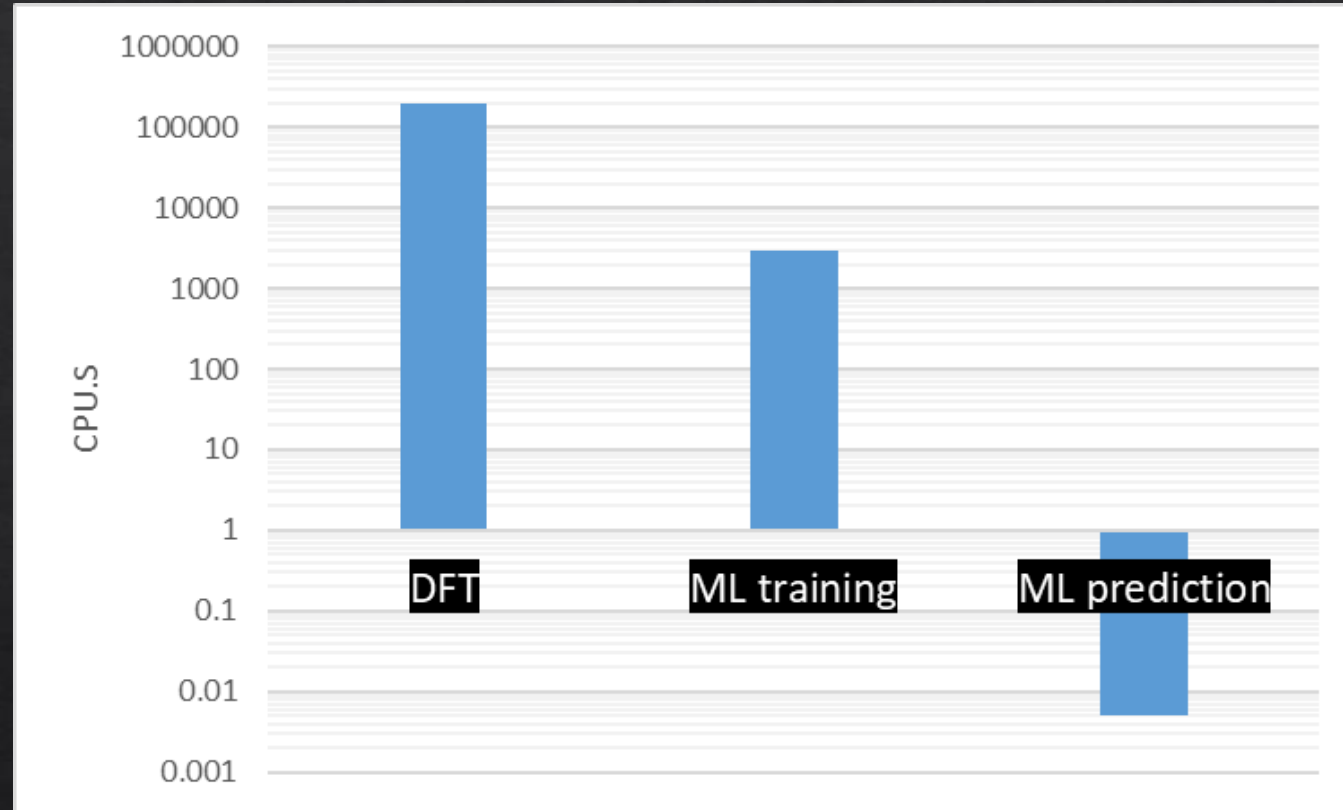
- ✓ Rotation



Dipole moment



Speed / Computational cost





Conclusions

- ❑ A rotationally equivariant descriptor for μ
- ❑ Prediction of μ and α using GPR
- ❑ Prediction of electric field forces using μ and α



Outlook

- Integration with LAMMPS
- Integration with FEMOCS
- Simulate the diffusion mechanism for tip growth
- Use on-the-fly machine learning



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- Andreas Kyritsakis
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Thank you for your attention!