Developing a Theoretical Understanding of Water Network Formation on Surface of Metal Oxides

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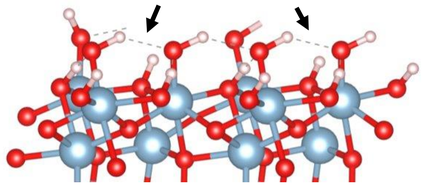
Research question: How does water arrange itself at diverse metal oxide-water interfaces?

Water Network Formation

Previous work done has shown that the arrangement of the water-network controls the surface chemistry. This project uses Density Functional Theory and Machine-Learned Force Fields to understand the water-network interactions.

Water H-Bond Network



Theoretical Background

Machine Learned Force Fields

- Gaussian Process to maps atomic environment descriptors to prediction of system energy and forces

Pros:

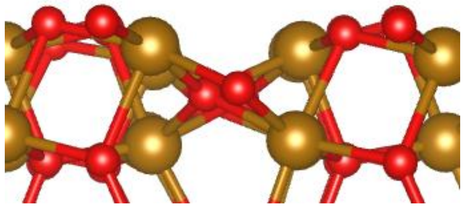
- Good for low-data, highly specialized machine learning

Cons:

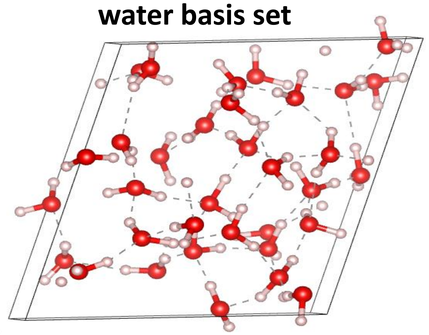
- Very memory intensive, large basis sets

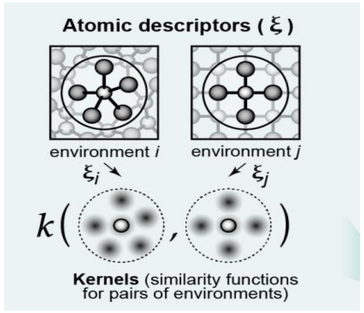
Methodology

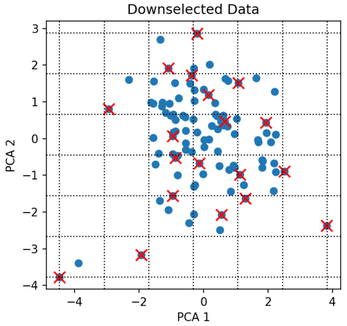
Create Target Structure



Generate large water-water basis set

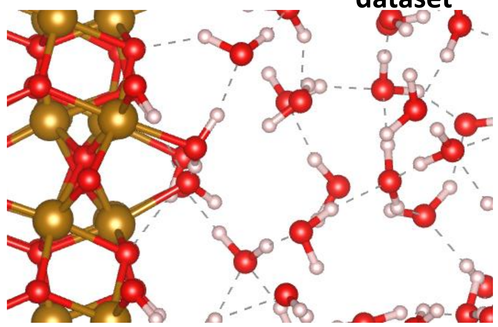






VASP MLFF on-fly-training

Downsize/optimize dataset



Combined surface+water

Preliminary Results

Successful

- Large dataset of water-water interactions has been created
- Basis set downselection via PCA has been implemented

Unsuccessful

- Complete methodology has not been fully implemented

Issues

Development of surface datasets

- Modelling of the magnetic ordering of AFM iron oxide (hematite) proved difficult
- Silica is modeled badly due to memory allocation issues

Conclusion and Future Work

- Finish implementing the complete methodology
- Compare to fully On-The-Fly approach

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