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.

Methodology

Create Target Structure

Generate large water-water basis set

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

Acknowledgments:
Dr. Muhich, Vivienne Pelletier, Muhich Lab, ASU FURI, TSMC

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

Water H-Bond Network

Theoretical Background
Machine Learned Force Fields

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