Abstract

Introduction

Fuel Cells

PEM fuel cell?

Overpotential?

Sabatiers Principle

Catalysis theory in general

Formic Acid Oxidation

Possible oxidation reactions (As Alexander showed in article)

Free energy diagrams

Modelling the activity of the two-step reaction

DFT machinery

Methods

Making data – show all Jack’s data and ref and my “own” data

Slabs for testing CO-OH slide reaction

Slabs for estimating H+COOH neighbor interactions

Slabs for estimating swim ring efficiency

Setting reference energies

Energy prediction models for adsorbate binding energies (With HEA and SWR data, hollow-site model, on-top model, mixed-site model) and all the equations and figures of them would be nice

Show a fcc(111) surface and hollow, on-top, mixed site

Using energy prediction models on simulated surfaces

Plotting them H vs COOH

Bayesian optimization of pair energies – searching for better composition

Coverage simulations and all the logic involved.

The random swim-ring mixture

Conclusion

Neighbor DFT data

Swim rings

Good composition found?

Method useful?

References

Notes about writing:

In Jack’s thesis he had these headlines between Introduction and Conclusion:

“Catalyst Discovery Using High-Entropy Alloys (?)

Calculating Adsorption Energies with Density Functional Theory (?)

Predicting DFT Adsorption Energies (?)

Optimizing the Composition (?)

Limitations of Methodology (?)”