Abstract

Introduction

Fuel Cells

PEM fuel cell?

Overpotential?

Formic Acid Oxidation

Possible oxidation reactions (As Alexander showed in article)

Free energy diagrams

Modelling the activity of the two-step reaction

Sabatiers Principle

Catalysis theory

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)

Using energy prediction models on simulated surfaces

Plotting them H vs COOH

Bayesian optimization of pair energies – searching for better composition

Coverage simulations

The random swim-ring mixture

Conclusion

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 (?)”