

Paper Analysis Notes

October 20, 2025

Authors

What fields are they from? How will that inform their approach to data collection, analysis, and interpretation?

The authors are doing theoretical surface science.

Summary

Provide a 2–3 sentence summary of the paper and what it is trying to communicate.

By considering the experimentally measured exchange current densities as a function of chemisorption energies, plots can be generated that form the shape of a volcano, where the top of the volcano is the sweet spot for catalysis. Then theoretical surface science tools are able to justify why this trend is observed, by giving a rigorous thermochemical answer.

Main points

What are the main points that the paper is trying to convey? What data is provided to support those points? What data is provided that may contradict/support alternative hypotheses? What additional data would help convey their points?

The paper is trying to convey that theoretical surface science is able to explain why certain metal electrodes catalyze HER better than others. They provide DFT calculations done with some local correlation-exchange functional to back up their claims. However, this type of DFT is known to have the band gap problem, so these volcano plots would carry more validity if a higher level of theory were used.

Motivation

What is the motivation for this paper? Is the motivation convincing, or do you think there are alternative motivations for this work?

It is experimentally observed that platinum is a good catalyst for many reactions, including HER. So the motivation for this paper is to show how theory can explain these trends.

Extraneous Information

What data is provided that is unnecessary to the main points of the paper? Are there specific figures or discussion points that should be moved from the main text to the SI? Is there

anything in the SI that should be moved to the main text?

It was a very short paper, so I don't think I have ideas about how to change the organization.

Flow

What jumped out to you (good or bad) about how this paper was written?

The paper was to the point, not including more details than necessary, so I thought this was good.

Future Directions

As researchers, we should always be thinking about next steps. What, if any, next papers should follow this one? Is there any additional analysis and conclusions that can be drawn from their data?

Doing a similar study, but with a higher level of theory, where computationally feasible.