

## Title

Old problem, new techniques: hydrogen evolution on Pt(111)

## Authors

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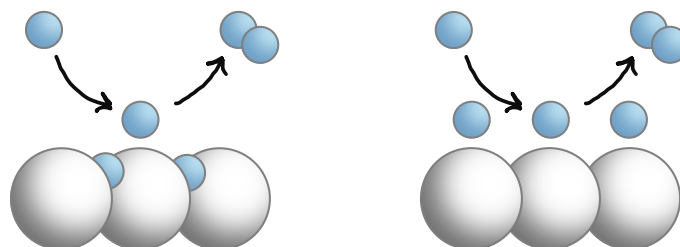
### Abstract poster presentation

The rate of the hydrogen evolution reaction on metal electrodes in aqueous electrolytes has traditionally been related to the hydrogen binding energy of the metal. Platinum electrodes give the highest reaction rate, but the reason why remains controversial: the binding energy of hydrogen depends significantly on the hydrogen adsorption site, and the hydrogen coverage.

Density functional theory calculations suggest that the platinum surface is covered by strongly-bound hydrogen in fcc-sites; occupation of top-sites is then unfavorable. Tafel slope analysis of experimental data requires that the reacting hydrogen species has a low coverage. The common interpretation is therefore that the fcc-hydrogens are inert, and that hydrogen evolution takes place on top-sites [1].

On the other hand, recent ab initio molecular dynamics studies [2, 3] suggest that under conditions where hydrogen evolution takes place, all hydrogen atoms reside on top-sites. Their discovery challenges the traditional paradigm, and should be verified with more accurate simulations.

A deeper understanding of where hydrogen atoms reside is needed to better understand the hydrogen evolution reaction, and ultimately to develop better catalysts. To study the behavior of adsorbed hydrogen atoms in more detail, we are developing a machine-learned interatomic potential for the platinum-water interface to efficiently run accurate molecular dynamics simulations. In this way, we can study various factors that affect the hydrogen configuration at the interface, and address computational shortcomings present in previous studies.



### Two possible hydrogen configurations during hydrogen evolution on a platinum surface

Left: the traditional picture, where the platinum surface is covered with hydrogen residing in fcc-sites.

Right: the picture based on recent ab initio molecular dynamics simulations, where the surface is covered with hydrogen residing on top-sites.

### References

1. Lindgren, P., et al. *A Challenge to the  $G \sim 0$  Interpretation of Hydrogen Evolution*. ACS Catal., 2020. **10**/1: p. 121-128. doi: 10.1021/acscatal.9b02799
2. Kronberg, R., et al. *Coupling Surface Coverage and Electrostatic Effects on the Interfacial Adlayer–Water Structure of Hydrogenated Single-Crystal Platinum Electrodes*. J. Phys. Chem. C, 2020. **124**/25, p. 13706–13714. doi: 10.1021/acs.jpcc.0c02323
3. Cucinotta, C., et al. *Revealing the Molecular Interplay of Coverage, Wettability, and Capacitive Response at the Pt(111)-Water Solution Interface under Bias*. Preprint, 2023. doi: 10.21203/rs.3.rs-3788305/v1