

Ad-hoc Design of Novel Catalytic Electrodes for High-Performance Hydrogen Fuel Cells

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Abstract

A recent push towards the hydrogen economy has renewed interest in proton exchange membrane fuel cells (PEMFCs). PEMFCs are suitable for portable usage such as light vehicles and heavy-duty transport vehicles on longer routes. The low operating temperature necessitates the utilization of noble metals such as platinum (Pt) to catalyse the redox reactions at desired rates to obtain enough power density. However, the high cost and scarcity of noble metals are among major issues in the way of widespread adoption of PEMFCs. This entails the pursuit of innovative ways to minimize the loading of noble metals and alternative solutions [1].

The electrochemical oxygen reduction reaction (ORR) is one of the major bottlenecks for the development of low-cost PEMFCs, as it involves multiple intermediates and reaction steps. The catalyst design strategies guided by the optimization of adsorption-free energies of ORR intermediates (*OOH, *O, and *OH) have been applied extensively owing to a direct relation with ORR overpotential. The binding energies can be tweaked by electronic and/or structural modifications in electrocatalysts. However, the adsorption energies are strongly correlated and change monotonically for different catalysts (Figure 2 A) [2], which limits the degrees of freedom for catalyst design and caps the performance of even noble metals at high overpotential. Herein, we will investigate how introducing heterogeneity to the catalyst surface alters the linear scaling relationships and enhances the overall performance of PEMFCs. Specifically, the combination of single or dual atom catalyst and interfacial electric field are investigated to overcome the ORR scaling relationship. Although all the ORR intermediates bind to surface through O atom giving rise to the linear scaling relationship, the application of interfacial electric field breaks the monotonic relationship of adsorption energies owing to different dipole moment and polarizability of ORR intermediates (Figure 2 B) [3].

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References

- [1] Jiao, K., Xuan, J., Du, Q. et al., Nature, 595 (2021) 361-369.
- [2] Kulkarni, A., Siahrostami, S., Patel, A., Nørskov, K., Chemical Reviews, 5 (2018) 2302-23012.
- [3] Wang, B., Wang, M., Fan, Z. et al., Nature Communication, 15 (2024) 1719.

Figures

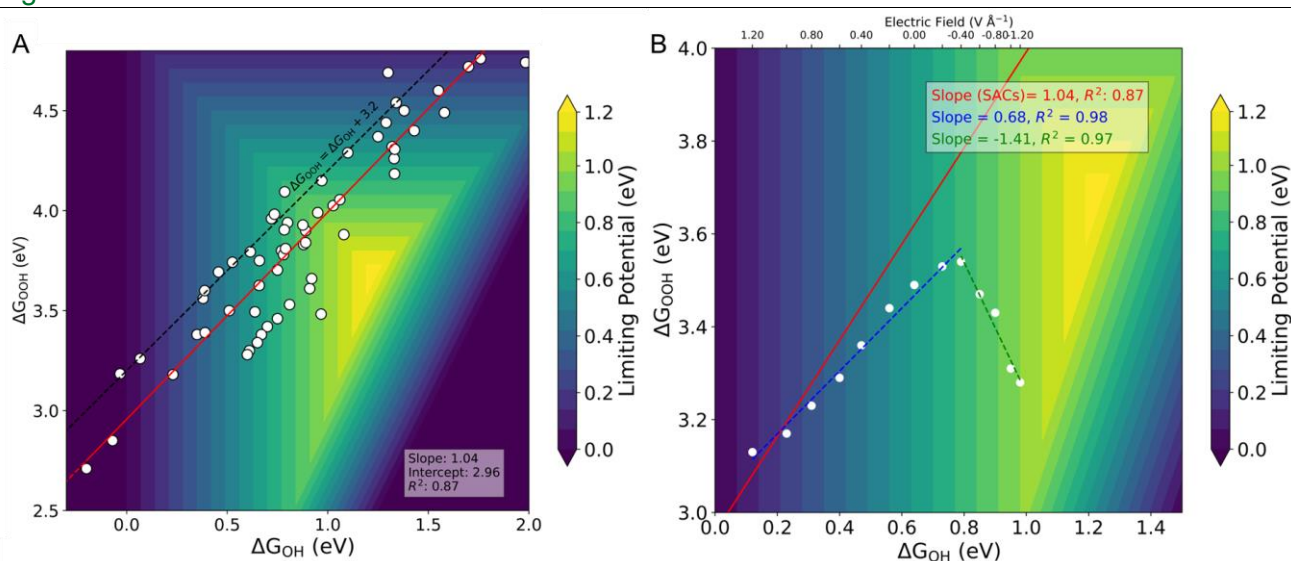


Figure 1: Scaling relationship of adsorption energy between *OH and *OOH intermediates. A) Deviation in ORR scaling relationship observed in single atom catalysts (SACs) (solid red line) from traditional nanoparticles (dotted black line [2]). B. Interfacial electric field modulates the $\Delta G(\text{OOH}^*)$ vs $\Delta G(\text{OH}^*)$ relationship in Fe-SACs [3].