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The combination of theory and experiment elucidates the remaining challenges in developing further improved catalysts, often involving scaling relations among reactive intermediates. This...

**Combining theory  
and experiment in  
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hydrogenation of  
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compounds on

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associated materials  
for several different  
electrochemical  
transformations  
involving water,  
hydrogen, and oxygen,  
using theory as a  
means to rationalize  
catalyst performance.

## **Combining theory and experiment in electrocatalysis ...**

Electrocatalysis: theory  
and experiment at the  
interface The need to  
develop

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cleaner/greener  
methods for both  
energy production and  
chemical synthesis has  
been generating  
renewed interest in  
electrocatalysis.

Experimental advances  
in the application of  
spectroscopic methods  
such as IR, INS, NMR,  
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meeting will bring  
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surface scientists and  
theoreticians together  
and foster the  
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electrocatalysts and associated materials for several different electrochemical transformations involving water, hydrogen, and oxygen, using theory as a means to rationalize catalyst performance.

## **Combining theory and experiment in electrocatalysis ...**

Theory and experiments join forces to characterize the



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electrocatalytic  
interface Stephan N.  
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PNAS April 16, 2019  
116 (16) 7611-7613;  
first published March  
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Electrocatalysis:  
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Design . Zhi Wei

Seh<sup>1,2,3</sup>, Jakob  
Kibsgaard<sup>1,2,4</sup>, Colin F.  
Dickens<sup>1,2</sup>, Ib

Chorkendorff<sup>4</sup>, Jens K.  
Nørskov<sup>1,2</sup>, Thomas F.  
Jaramillo<sup>1,2\*</sup> Abstract .

Electrocatalysis plays a  
central role in clean  
energy conversion,  
enabling a number of  
sustainable

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Experiments to directly measure the interface behavior and test the theory/simulations are challenging because conventional photoelectrochemical techniques do not measure the electrocatalyst potential during operation. We developed dual-working-electrode (DWE) photoelectrochemistry to address this

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limitation.

## **Semiconductor-Electrocatalyst**

### **Interfaces: Theory ...**

Returning to the Netherlands in 1997, I found an almost ideal environment to combine theory and experiment in electrocatalysis in Rutger van Santen's group at Eindhoven, as combining theory and experiment was the group's claim to fame

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## **Combining experiment and theory for understanding ...**

Analyzed  
contradictions between  
theory and experiment.

- Process of activation  
of ORR and OER still  
not resolved. •

Advancement in  
oxygen electrocatalysis

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requires understanding of activation entropy. • Focus on interfacial electrocatalytic descriptors and interfacial water structure. • Besides electrocatalysis, crucial is knowledge ...

**Is a major  
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oxygen  
electrocatalysis ...**

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