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Combining Theory and Experiment in Electro catalysis: Insights into Materials 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 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 in the world of heterogeneous catalysis and surface science.

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

## **Is a major breakthrough in the oxygen electrocatalysis ...**

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