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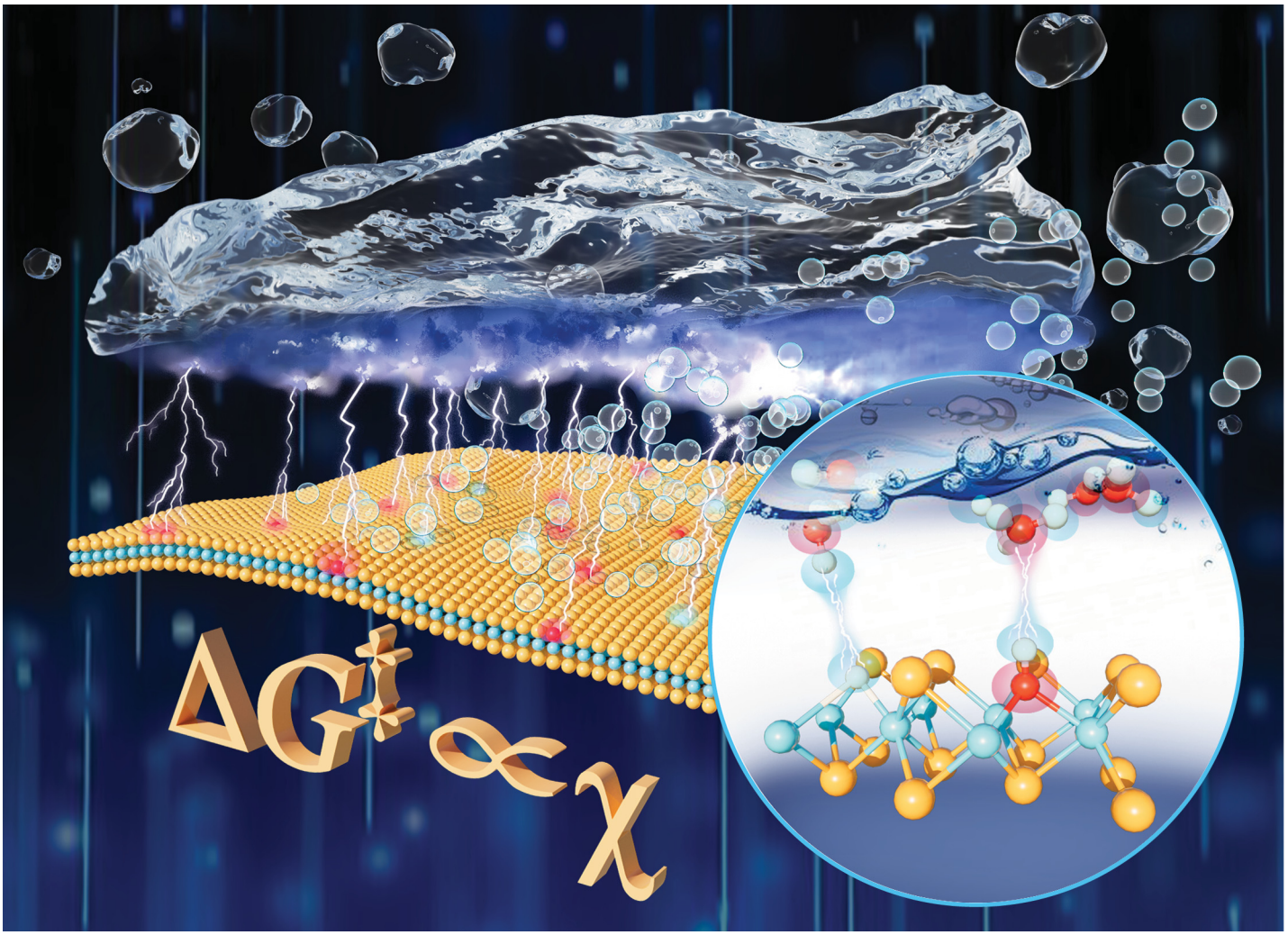
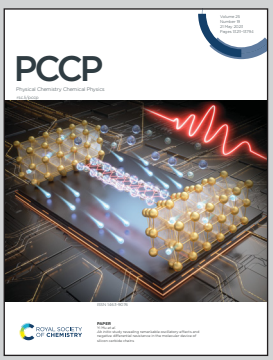


Showcasing research from the Group of Prof. Xiaobo Chen at Jinan University, China

Electronegativity principle for hydrogen evolution activity using first-principles calculations

This work reports a positive correlation between the reaction kinetics and interfacial charge transfer for the hydrogen evolution reaction. The charge transfer can be well captured by the Mulliken electronegativity χ of a catalyst because the reaction barrier shows a linear dependence on χ for a wide range of catalysts. A catalyst with lower electronegativity exhibits a lower barrier and thus a faster reaction rate. This electronegativity principle is reaction route and pH independent and is founded on the thermoneutral requirement on ΔG_{H}.

As featured in:



See Xiaobo Chen *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 13289.

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