Breaking electrochemical scaling laws in atomically engineered van-der-Waals stack multisite edge catalysts

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Abstract

Electrocatalysis is key to sustainable energy conversion and storage, but its efficiency is limited by scaling laws between reactant adsorption and desorption. Multisite catalysts promises to overcome these limits, but challenges in fabrication and characterization hinder its validation. We present a platform to study and optimize multisite electrocatalysis. Leveraging van der Waals stacked 2D materials, we create catalytic edge assemblies with precise activity variations, enabling atomically engineered site separation and interaction. This approach enables the identification of multisite catalysts that enhance the hydrogen evolution reaction (HER) beyond single-site Sabatier scaling. Altering atomic-scale site separations reverts the system to single-site mechanisms, highlighting the importance of intermediate transport. Direct evidence of intermediate exchange is provided by electrostatic control of the sites, supported by ab initio simulations. We further engineer bifunctional catalysts for the oxygen evolution reaction (OER) and HER, achieving superior neutral water splitting. These findings enable the catalytic cascade design and complex electrochemical synthesis.[1] (Figure 1)

References

[1] D.-R. Chen, J. Muthu, J.-T. Chang, P.-H. Lin, Y.-X. Chen, F. Khurshid, H.-T. Chin, J. Kong, M. Hofmann, and Y.-P. Hsieh, Nano Letters, 31 (2025) 12059–12066

Figures

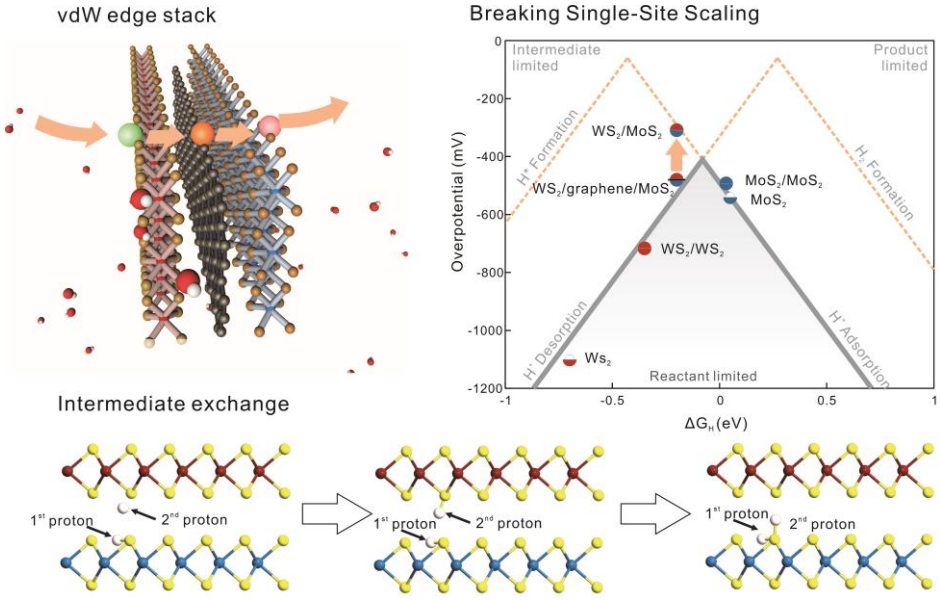

Figure 1: The figure illustrates multisite vdW edge-stack catalysis, in which atomic-level control of site separation and interaction enables intermediate exchange and breaks the single-site Sabatier scaling.