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Catalyst Design for Net-Zero Hydrogen Production:
Breaking Activity–Stability Trade-Offs

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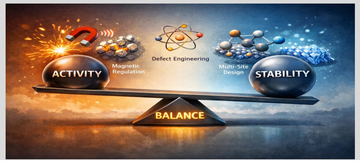
Introduction

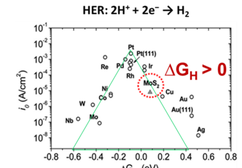
Highly active sites tend to be unstable, while stable structures often lack sufficient activity. To bridge this gap, we develop three synergistic catalytic strategies for net-zero hydrogen and renewable carbon cycling:

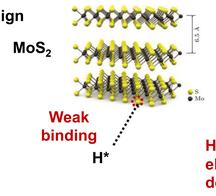
- **Spin regulation via ferromagnetic graphene**
  Spin-polarised HER energetics and kinetics
- **Multi-site catalysis for chemical hydrogen release**
  Cooperative Pt single atom–Ni cluster pathways



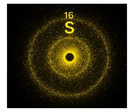
I · Spin-Regulated HER Catalysis (Ferromagnetic graphene modulates hydrogen adsorption)

Theory guidance for HER catalysts design



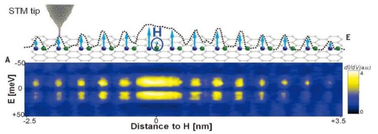


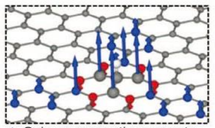
Active sites



High electron density

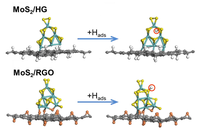
The ferromagnetism of Hydrogenated Graphene





- unpaired electrons
- delocalized π bonding network

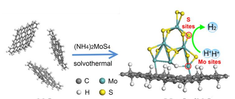
DFT: Hydrogen adsorption energy

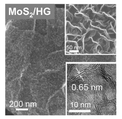


Catalysts	E_{ads} (eV)
Pt	−3.30
MoS_2/HG	−2.79
MoS_2/RGO	−2.22
Without ferromagnetism	−2.13

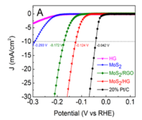
HG weakens the electron-rich state of S & optimizes hydrogen adsorption energy of MoS_2 during HER

Preparation of MoS_2/HG

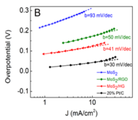




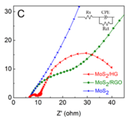
Activity



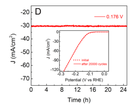
Kinetics



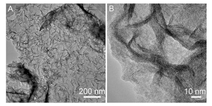
Interface reactions



Durability & stability

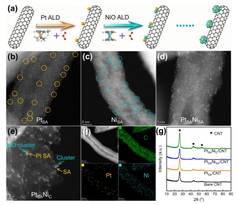


Structural stability



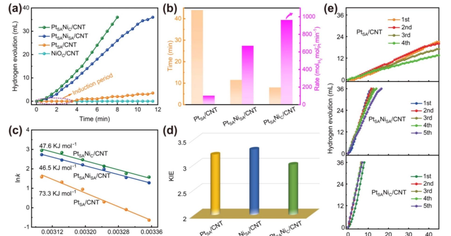
II · Multi-site Catalysis for Ammonia Borane Dehydrogenation (Pt single atom–Ni cluster interfaces)

$Pt_{SA}Ni_C$/CNT

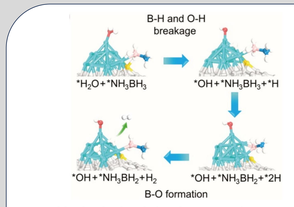


Atomically engineered platinum single atom-nickel cluster synergistic interfaces

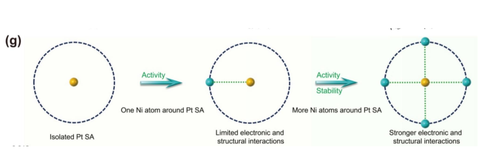
Activity and durability evaluation



Ammonia borane dehydrogenation reaction (0.05 mol L^{-1} AB, 20 mg of catalysts, 25 °C)



Hydrolytic dehydrogenation process over the representative $Pt_{SA}Ni_C$/CNT catalyst.



Schematic presentation of Pt-Ni interactions.

H_2 evolution activity and durability over the representative Pt_{SA}/CNT and $Pt_{SA}Ni_C$/CNT catalysts

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References:

1. Xiuxiu Han, et al., ACS Catalysis. 2018, 8, 1828-1836.
2. Xiuxiu Han, et al., Science Bulletin. 2026, 71, 1357–1368.