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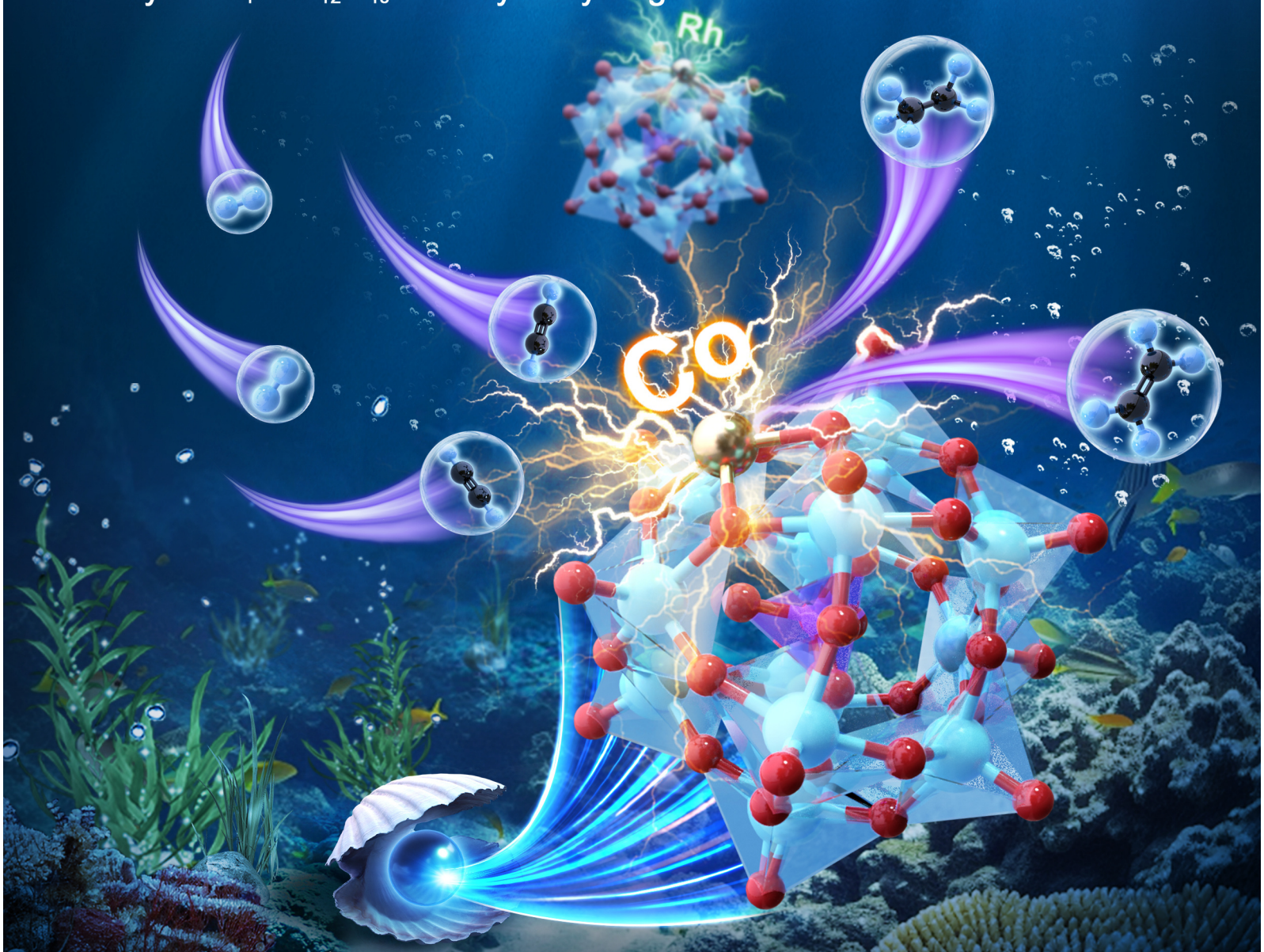
Theoretical catalytic performance of single-atom catalysts $M_1/PW_{12}O_{40}$ for alkyne hydrogenation materials



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Perspective

Highlights

Transfer learning prediction on lithium-ion battery heat release under thermal runaway condition

Changmin Shi[1,*], Di Zhu[2], Liwen Zhang[3], Siyuan Song[1], and Brian W. Sheldon[1]

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Research Articles

Front Cover

Theoretical catalytic performance of single-atom catalysts $M_1/PW_{12}O_{40}$ for alkyne hydrogenation materials

Shamraiz Hussain Talib[2], Xuelian Jiang[3], Shixiang Feng[4], Mengdie Zhao[1], and Qi Yu[1,3,*]

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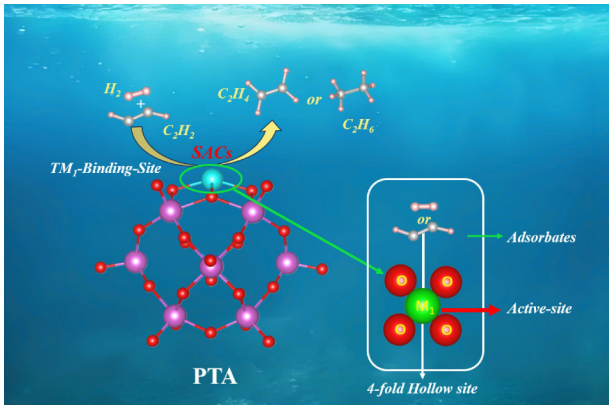

This work significantly advances catalytic mechanisms for alkyne hydrogenation to alkene under ambient conditions, emphasizing the effectiveness of Rh_1/PTA single-atom catalyst and offering valuable insights for the development of sustainable and efficient catalytic processes.

Robust ring insoluble naphthoquinone derivative cathode with high loading and long cycle life for aqueous zinc organic batteries

Jiali Wang[1], Xinyu Gao[1], Yongwen Wang[1], Ruonan Pan[1], Zhen Liu[1], Xin Liu[1], Haijiao Xie[2], Feng Yu[1], Gang Wang[1,*], and Tiantian Gu[1,*]

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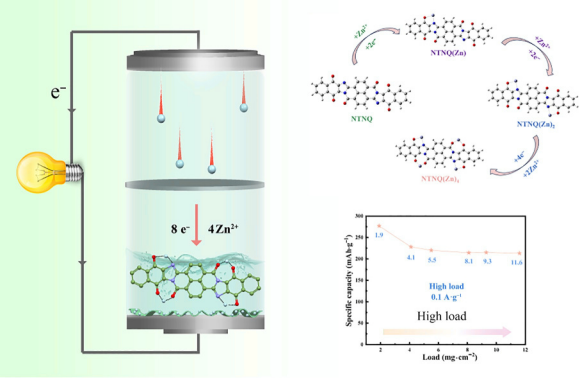

The synergistic effect of neighboring active sites and multi-electron Zn^{2+} storage reactions are explored by DFT calculations, and the results suggest that NTNQ could stores $4Zn^{2+}$ while transferring $8e^-$ in the N-Zn-O pathway during the storage of Zn^{2+}. And, NTNQ still exhibits high specific capacity and favorable cycling stability at multiple ultra-high loadings. The design concept of organic molecules and the investigation of Zn^{2+} storage mechanism in this work provide new opportunities for the future synthesis of high-energy aqueous zinc organic batteries.

Pre-doped cations in V_2O_5 for high-performance Zn-ion batteries

Yinan Lu[1], Tianlei Wang[2], Nibagani Naresh[1], Joanna Borowiec[2], Ivan P. Parkin[2,*], and Buddha Deka Boruah[1,*]

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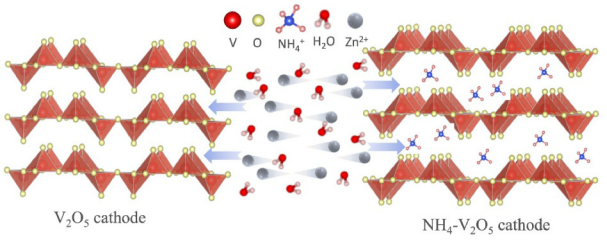

This study examines how pre-cation doping significantly impacts the capacity response of V_2O_5 cathode materials in Zn-ion batteries. It explores the effects of pre-doping with various cations (including Na^+, K^+, and NH_4^+) on enhancing overall charge storage performance.

A tailored highly solvating electrolyte toward ultra lean-electrolyte Li–S batteries

Zixiong Shi[1], Simil Thomas[2], Zhengnan Tian[1], Dong Guo[1], Zhiming Zhao[1], Yizhou Wang[1], Shuo Li[1], Nimer Wehbe[3], Abdul-Hamid Emwas[3], Osman M. Bakr[1], Omar F. Mohammed[2], and Husam N. Alshareef[1,*]

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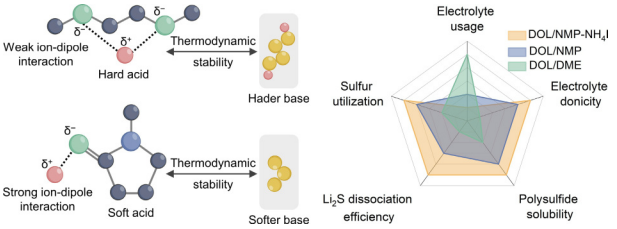

High-donicity DOL/NMP-NH_4I electrolyte is developed to elevate the sulfur utilization and electrochemical performance Li–S batteries especially under lean-electrolyte condition. We correlate the solvation structure, polysulfide speciation, Li_2S nucleation behavior and lean-electrolyte battery performance with donicity and denticity of electrolytes. Li–S batteries with a starved *E/S* ratio of 3 $\mu L \cdot mgs^{-1}$ and a high sulfur loading of 4 $mg \cdot cm^{-2}$ can sustain a stable operation over 30 cycles.

A self-healing aqueous ammonium-ion micro batteries based on PVA-NH_4Cl hydrogel electrolyte and MXene-integrated perylene anode

Ke Niu[1,2], Junjie Shi[2], Long Zhang[2], Yang Yue[3], Mengjie Wang[3], Qixiang Zhang[2], Yanan Ma[4], Shuyi Mo[1], Shaofei Li[1], Wenbiao Li[1], Li Wen[2], Yixin Hou[1], Fei Long[1,*], and Yihua Gao[1,2,*]

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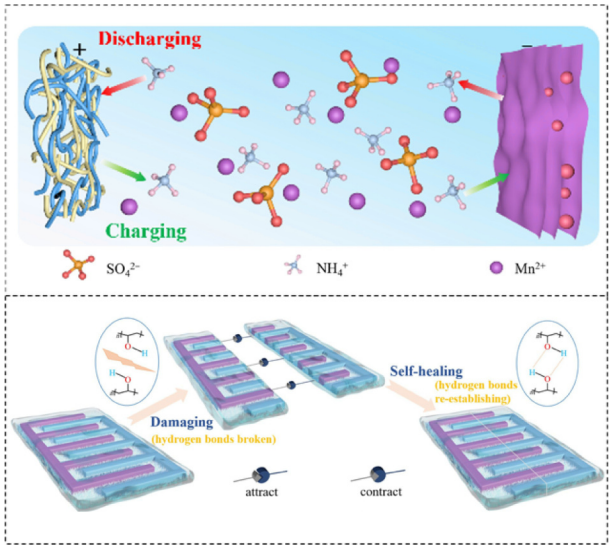

The first self-healing aqueous NH_4^+ micro batteries (AMBs) are reported, assembled by PVA-NH_4Cl hydrogel electrolyte, PTCDI-MXene anode and MnO_2-CNTs cathode. The AMBs exhibit excellent cycle life, flexibility, self-healing ability, energy density and power density, providing a new option for the next generation of micro flexible-energy storage devices.

FeCoP sub-nanometric-sheets for electrocatalzing overall water splitting

Long Zhao[1], Kexin Meng[1], Yibo Guo[2], Qingsheng Wu[1], Quanjing Zhu[1], Tao Zhou[1], Yongqing Fu[3], and Ming Wen[1,*]

[1] School of Chemical Science and Engineering, School of Environmental Science and Engineering, Shanghai Key Laboratory of Chemical Assessment and Sustainability, State Key Laboratory of Pollution Control and Resource Reuse, Tongji University, Shanghai 200092, China
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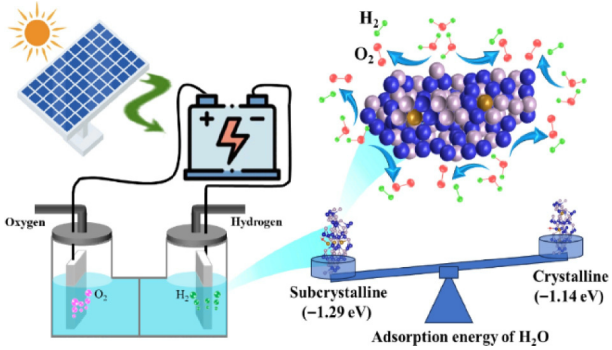

The application of renewable electric energy, converted from solar power, to electrolysis water systems, wherein as-synthesized subcrystalline FeCoP ultrathin nanostructure with abundant active sites and optimized d-electronic configurations of Co were used as bifunctional catalyst. The system realizes a completely green industrial chain for hydrogen energy.

Tuning electrochemical properties of carbon nanofiber electrodes with selenium heteroatoms for flexible zinc ion capacitors

Wenjie Liu, Fen Qiao*, and Jikang Zhao

School of Energy & Power Engineering, Jiangsu University, Zhenjiang 212013, China

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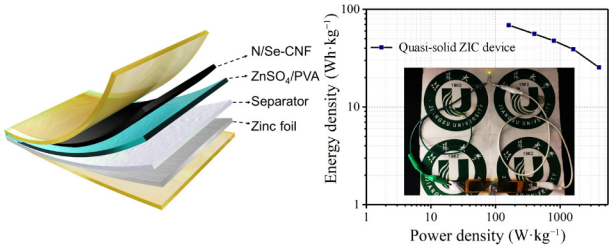

Se heteroatom doped N-rich carbon nanofibers (N/Se-CNF) have been synthesized using electrospinning to produce a superior electrode for flexible zinc ion capacitors (ZICs). The high level of N doping enhances the hydrophilicity and graphitization degree of CNF. The inclusion of Se heteroatom in carbon-based materials not only enhances their pseudocapacitance but also reduces the presence of pyrrole N, thus improving the electrochemical kinetics of the electrode. ZIC and quasi-solid flexible ZIC, composed of N/Se-CNF electrodes, demonstrate a notable energy density of 95.3 $Wh \cdot kg^{-1}$ (at 160.1 $W \cdot kg^{-1}$) and 68.8 $Wh \cdot kg^{-1}$ (at 160 $W \cdot kg^{-1}$) correspondingly, alongside exceptional electrochemical reversibility. This research offers a pioneering approach and theoretical framework for exploring dual-atom doping and governing N doping entities.

Back Cover

Boosting oxygen evolution performance over synergistic tiara nickel clusters and thin layered double hydroxides

Xinrui Gu[1,5], Song Guo[1], Yifei Zhang[2], Jingjing Zhang[1], Piracha Sanwal[1], Liangliang Xu[3,*], Zhen Zhao[2,*], Rongchao Jin[4], and Gao Li[1,2,5,*]

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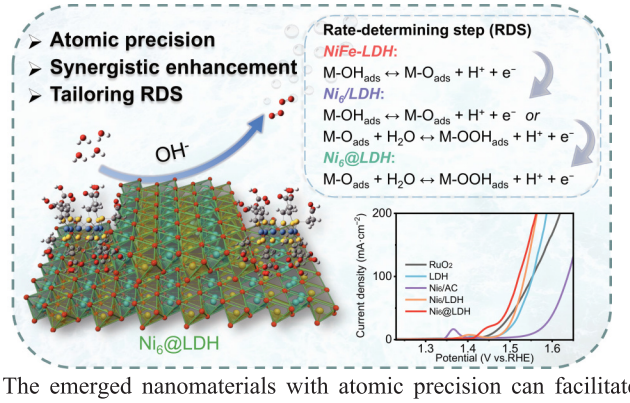

The emerged nanomaterials with atomic precision can facilitate joint experimental and computational studies in energy conversions. The synergistic Ni_6 clusters combined with LDH nanosheets mediate the rate-determining step in oxygen evolution reaction.

Review Articles

Piezoelectricity and triboelectricity enhanced catalysis

Nianzu Liu[1,*], Ruoxing Wang[2,*], Jiawei Zhao[3], Jing Jiang[2,4,*], and Feng Ru Fan[3,*]

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[3] State Key Laboratory of Physical Chemistry of Solid Surfaces, iChEM, College of Chemistry and Chemical Engineering, Innovation Laboratory for Sciences and Technologies of Energy Materials of Fujian Province (IKKEM), Xiamen University, Xiamen 361005, China
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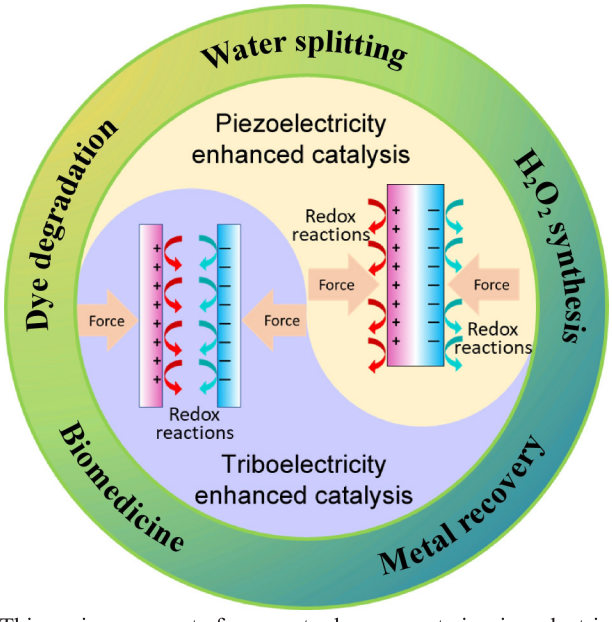

This review accounts for recent advancements in piezoelectricity and triboelectricity enhanced catalysis, covering basic understandings, catalyst design, and performance insights. Finally, challenges and future opportunities for piezoelectricity and triboelectricity enhanced catalysis are discussed.

Advances and prospects of g-C_3N_4 in lithium-sulfur batteries

Hong Yin[1,2,*], Jin He[1], Bo Xiao[1], Miao Zhou[1], Wei Wang[1], Joao Cunha[2], Zuxin Chen[3], Zhaohui Hou[1], Tianqi Zhang[2,4,*], and Zhipeng Yu[2,*]

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[2] International Iberian Nanotechnology Laboratory (INL), Av. Mestre Jose Veiga, 4715-330 Braga, Portugal
[3] School of Semiconductor Science and Technology, South China Normal University, Foshan 528225, China
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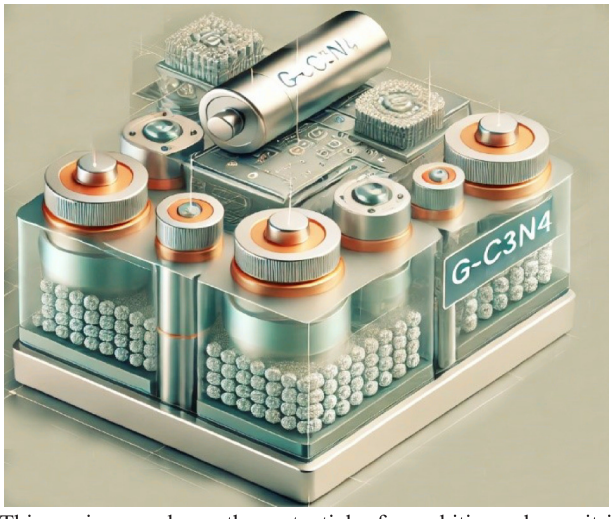

This review explores the potential of graphitic carbon nitride (g-C_3N_4) to overcome key challenges in lithium-sulfur (Li-S) batteries, such as the shuttle effect, low conductivity, and volume expansion. It focuses on the modification of g-C_3N_4 through defect engineering and nanocrystallization, as well as its compounding with metals, non-metals, graphene, porous carbon, and heterojunctions. The review aims to provide new insights and strategies for the rational design of g-C_3N_4 materials to optimize their application in Li-S batteries.

AIMS & SCOPE

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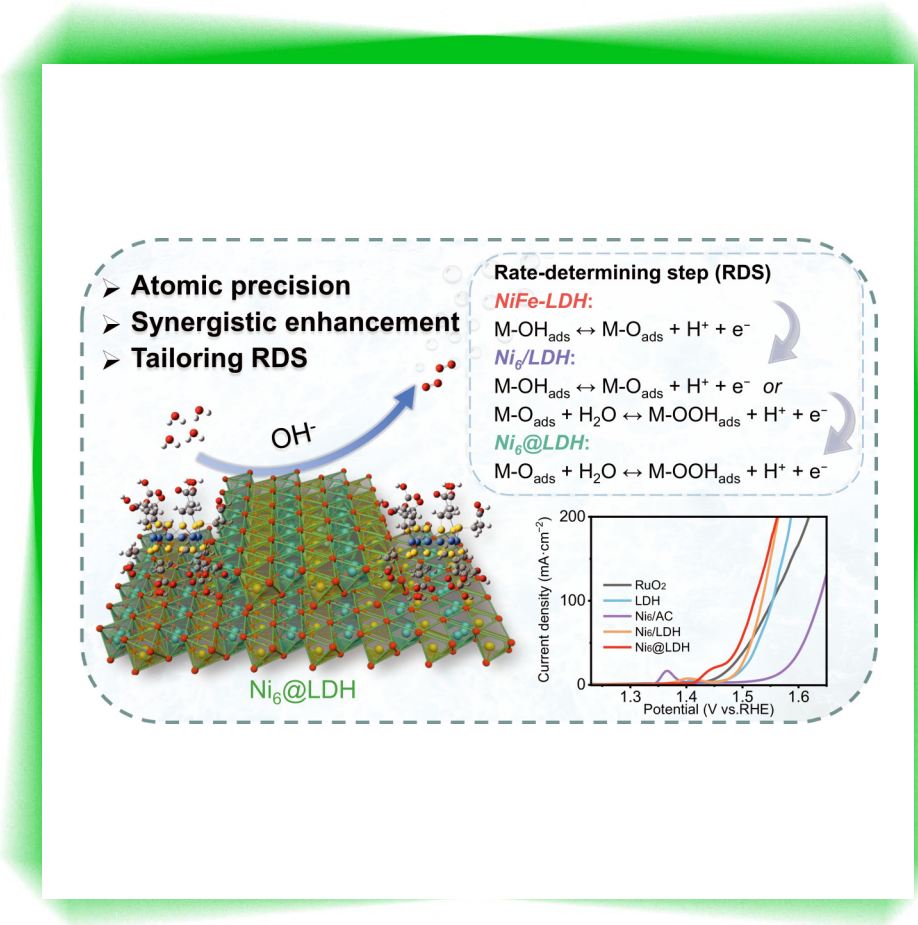

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