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應用物理及材料工程研究院
INSTITUTO DE FÍSICA APLICADA E ENGENHARIA DE MATERIAIS
INSTITUTE OF APPLIED PHYSICS AND MATERIALS ENGINEERING

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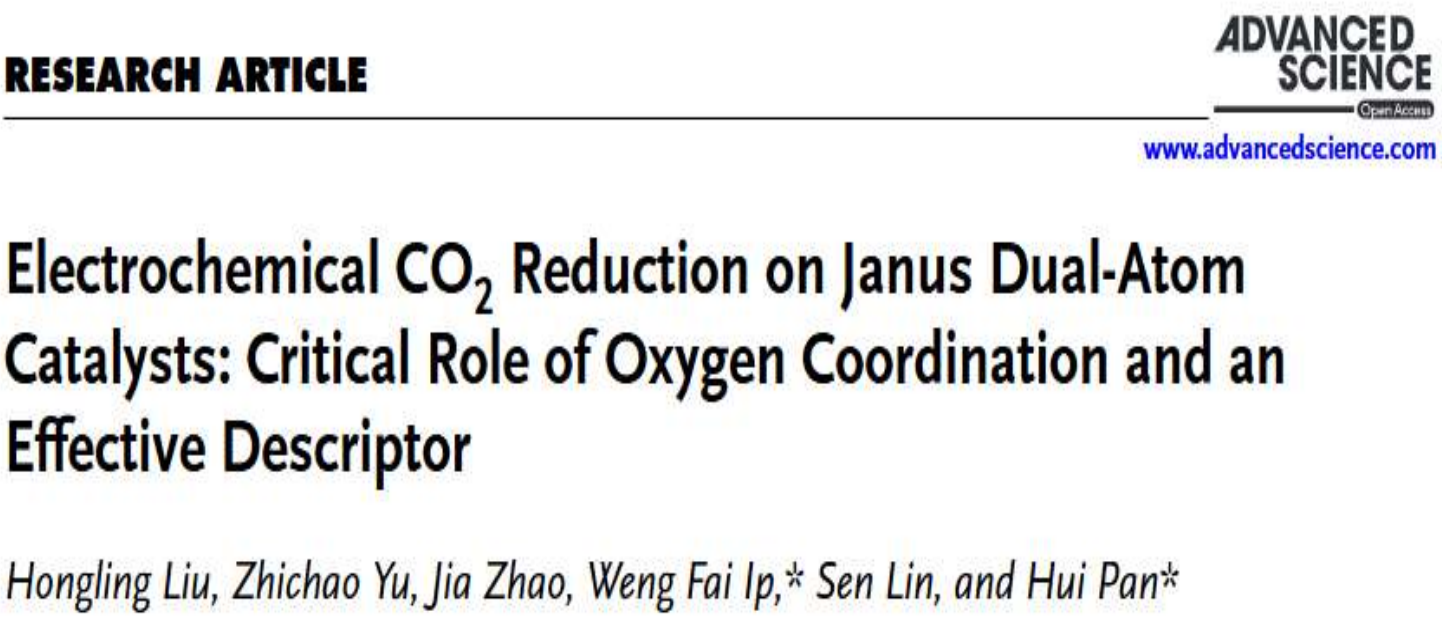
✧ Content

❖ Publications (IF≥8, and/or nature Index; *corresponding author)

1. **Hongling Liu**, Zhichao Yu, Jia Zhao, Weng Fai Ip*, Sen Lin, and **Hui Pan***. Electrochemical CO_2 Reduction on Janus Dual-Atom Catalysts: Critical Role of Oxygen Coordination and an Effective Descriptor. *Advanced Science*, e07849 (2025). DOI: 10.1002/advs.202507849. [2024 IF=14.1]



RESEARCH ARTICLE

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Electrochemical CO_2 Reduction on Janus Dual-Atom Catalysts: Critical Role of Oxygen Coordination and an Effective Descriptor

Hongling Liu, Zhichao Yu, Jia Zhao, Weng Fai Ip, Sen Lin, and Hui Pan**

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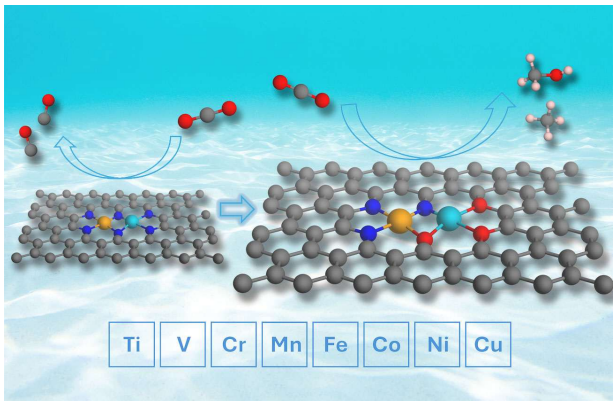
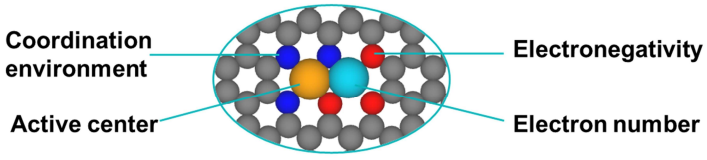
❖ Research Stories

UM research team demonstrates critical role of oxygen coordination in Janus dual-atom catalysts for electrochemical CO2 reduction and proposes an effective descriptor

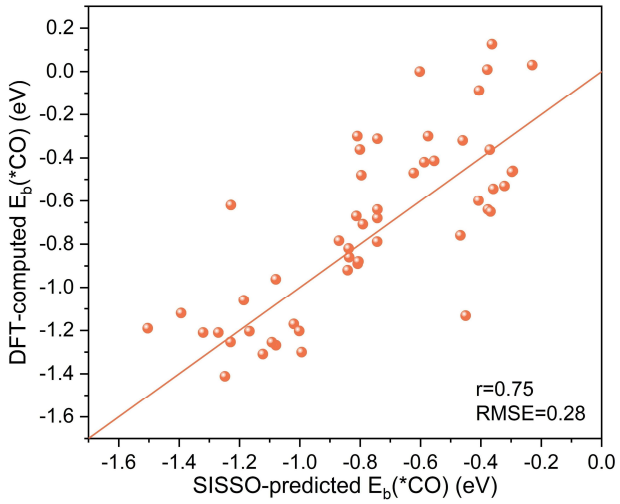
- Electrocatalytic carbon dioxide reduction (CO_2R) is an appealing approach to alleviate the greenhouse effect and achieve carbon-neutral circulation. The widely studied dual-atom catalysts (DACs) embedded in nitrogen-doped graphene are effective for electrochemical CO_2R to CO. However, their selectivity for C1 hydrocarbons remains a challenge.
- The team designed Janus DACs (J-M'M) with partial oxygen coordination for converting CO_2 to methanol and methene by first-principles calculations and illustrated the underlying mechanism by comparing with the normal DACs (N-M'M).
- In contrast to normal DACs, most Janus DACs tend to produce CH_3OH or CH_4 instead of CO due to their stronger *COOH and *CO binding strength. With the constant-potential calculations, J-FeCo and J-CoNi exhibit superior CO_2R activity to produce the CH_3OH and CH_4 with the favorable limiting potential of −0.38 and −0.45 V vs. RHE, respectively. Oxygen coordination in J-FeCo and J-CoNi regulate majority-/minority-spin energy levels of d_{z2}, d_{yz}, and d_{xz} orbitals toward the Fermi level, thereby improving CO adsorption. Based on the intrinsic atomic properties, an effective descriptor (φ) was identified to predict the *CO adsorption energy of Janus DACs for the prediction of potential Janus DACs with high catalytic performance.

Hongling Liu (劉虹伶) Prof. Hui Pan (潘暉) Prof. Weng Fai Ip (葉穎暉, FST)





$$\varphi = 0.00367 \frac{Nd}{\frac{\chi_{M/M'}}{\chi_{O/N}} - \frac{\chi_{M'/M}}{\chi_{N/O}}} - 0.765$$



Hongling Liu, Zhichao Yu, Jia Zhao, Weng Fai Ip*, Sen Lin, and Hui Pan*. Electrochemical CO_2 Reduction on Janus Dual-Atom Catalysts: Critical Role of Oxygen Coordination and an Effective Descriptor. *Advanced Science*, e07849 (2025). DOI: 10.1002/advs.202507849. [2024 IF=14.1]

The first author is Ms. Hongling Liu, Ph.D. student in the IAPME. This work was supported by the Science and Technology Development Fund (FDCT) from Macau SAR (0050/2023/RIB2, 0023/2023/AFJ, 006/2022/ALC, 0087/2024/AFJ and 0111/2022/A2), and Multi-Year Research Grants (MYRG-GRG2024-00038-IAPME, and MYRG-GRG2023-00010-IAPME) from the University of Macau.

❖ Seminars

On September 15, 2025, Prof. Francis Chi-Chung Ling (凌志聰) from the University of Hong Kong visited our institute to deliver a seminar entitled "*Defect Engineering of Functional Materials*". Hosted by Prof. Shuang-Peng Wang, the event attracted faculty members, researchers, and students, fostering a dynamic exchange of ideas at the forefront of materials science.

Prof. Ling, a tenured Associate Professor at HKU and a Fellow of the Institute of Physics (U.K.), is internationally recognized for his contributions to defect characterization and functionalization in materials physics. With a distinguished academic background—BSc, MPhil, and PhD from HKU—Prof. Ling has held several key academic and administrative roles, including Associate Dean of the Faculty of Science and Senate Member at HKU. His prolific research output includes over 204 SCI journal publications and more than 4,500 citations, focusing on defect control for optimizing material performance and device applications.

During his lecture, Prof. Ling highlighted the pivotal role of atomic-scale defects in tuning the electrical, optical, magnetic, and dielectric properties of functional materials. He presented three case studies:

- Enhancing oxide permittivity through the formation of acceptor-donor defect complexes
- Achieving a 30-fold reduction in leakage current in SiC junction barrier Schottky diodes via defect manipulation
- Modulating luminescence intensity and saturated magnetization in Cu-doped ZnO by controlling defect level occupancy

The presentation sparked lively discussions among attendees, who engaged Prof. Ling with questions on both fundamental mechanisms and practical applications.

Following the seminar, Prof. Ling toured the institute's laboratories, guided by Prof. Wang. He engaged in in-depth discussions with researchers and students, exploring avenues for future collaboration. Prof. Ling's visit and lecture provided valuable insights into defect engineering, reinforcing the institute's commitment to advancing research and fostering academic exchange in materials science.