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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

IAPME Newsletter

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ISSUE 56

15 October 2025

✧ Content

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

1. **Guanping Xu, Zirui Zhao**, Zhong Lin Wang, and **Hai-Feng Li***. Integrating machine learning with triboelectric nanogenerators: Optimizing electrode materials and doping strategies for intelligent energy harvesting. *Nano Energy* **142**, 111131 (2025). DOI: 10.1016/j.nanoen.2025.111131. [2024 IF=17.1]

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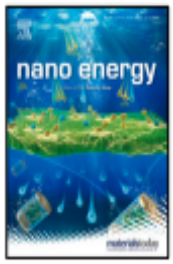

Full paper

Integrating machine learning with triboelectric nanogenerators: Optimizing electrode materials and doping strategies for intelligent energy harvesting

Guanping Xu [a,1], Zirui Zhao [a,1], Zhong Lin Wang [b], Hai-Feng Li [a,*]

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❖ Research Stories

UM Research Team Pioneers Machine Learning to Unlock High-Performance Energy Harvesting Materials

- This study introduces a robust machine learning framework that utilizes Graph Neural Networks (GNNs) to predict and optimize the performance of triboelectric nanogenerators (TENGs). The model accurately forecasts optimal electrode materials and doping strategies, achieving unprecedented accuracy in predicting key performance metrics like energy density.

- The data-driven approach led to the discovery of highly effective material combinations, such as PTFE doped with 7% silver, predicted to achieve a remarkable energy density of 1.12 J/cm^2. Experimental validation confirmed the model's high accuracy, with performance improvements of up to 85.7% for certain doped polymers.

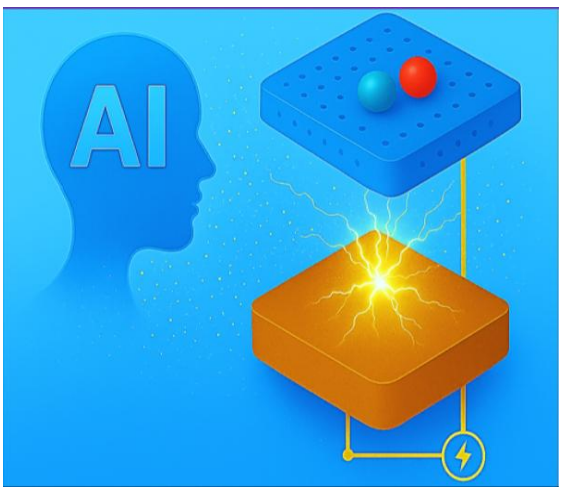
- This methodology establishes a new paradigm for intelligent material design, significantly accelerating the discovery of high-performance materials for TENGs while reducing reliance on costly and time-consuming experimental trials. It provides a powerful platform for advancing sustainable energy harvesting technologies and self-powered systems.

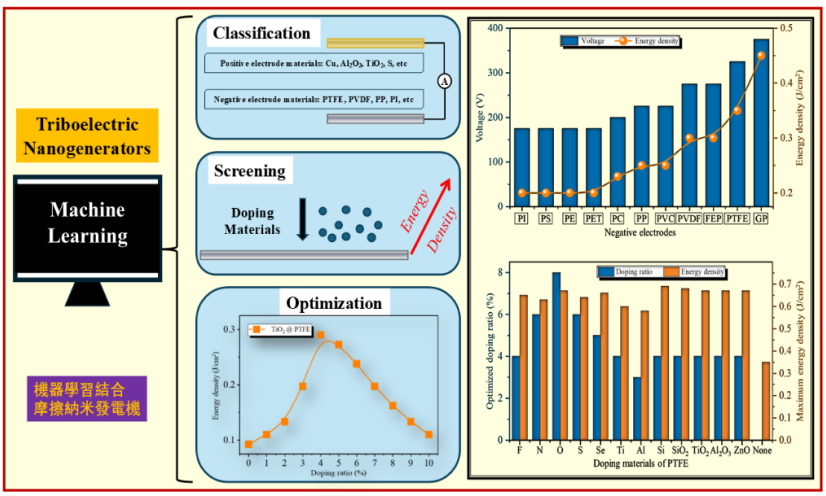
Mr. Guanping Xu
(徐官平)

Mr. Zirui Zhao
(趙梓睿)

Prof. Zhong Lin Wang
(王中林, UCAS)

Prof. Hai-Feng Li
(李海峰)





Guanping Xu, Zirui Zhao, Zhong Lin Wang, and **Hai-Feng Li***. Integrating machine learning with triboelectric nanogenerators: Optimizing electrode materials and doping strategies for intelligent energy harvesting. *Nano Energy* **142**, 111131 (2025). DOI: 10.1016/j.nanoen.2025.111131. [2024 IF=17.1]

Guanping Xu and Zirui Zhao, Ph.D. students in the IAPME, contributed equally. This work was supported by the Science and Technology Development Fund, Macao SAR (File Nos. 0104/2024/AFJ and 0115/2024/RIB2), University of Macau (MYRG-GRG2024-00158-IAPME), and the Guangdong-Hong Kong-Macao Joint Laboratory for Neutron Scattering Science and Technology (Grant No. 2019B121205003).

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❖ Institute Showcased the Research and Product at the 11th Macau Industrial Products Show

Our institute participated in the 11th Macau Industrial Products Show, held from October 2 to 5, 2025, where we presented a selection of our latest research innovations to the public.

Among the highlights were two pioneering research products that drew considerable attention from attendees:

- **Skin-Repairing Hydrogel Based On Carbon Quantum Dots**, developed by Prof. Songnan Qu (曲松楠), offering promising applications in biomedical technology.
- **Polymer/Cement Nanocomposite Materials**, developed by Prof. Guoxing Sun (孫國星), aimed at enhancing the performance of construction materials.

Throughout the four-day exhibition, our booth welcomed visits from students and teachers representing more than ten secondary schools across Macau. The engagement provided a valuable opportunity for young learners to explore cutting-edge scientific advancements and interact with researchers.

Our institute has maintained a strong presence at the Macau Industrial Products Show over the years, consistently showcasing our latest research and translational achievements. This ongoing participation reflects our commitment to fostering public understanding of materials innovation and strengthening collaboration between academia and industry.

❖ Upcoming Events

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IAPME Seminar

Electroreduction Reaction Mechanism of Metal-nitrogen-carbon Catalysts through Numerical Simulations

17 October 2025

Prof. Shuzhou LI
Nanyang Technological University
Venue: N23-3022
Time: 10:30 - 11:30
Hosted by: Prof. Yongqing CAI

Abstract

With the rapid progress in computer science, numerical simulations, including density functional theory and molecular dynamics simulations become an important approach in physical science. With density functional theory calculations, we explored reaction mechanisms of electrochemical reactions, such as oxygen reduction and CO_2 reduction that play an important role in energy conversion and energy storage. Single-atom iron embedded in N-doped carbon (Fe-N-C) is among the most representative single-atomic catalysts (SACs) for electrochemical CO_2 reduction reaction (CO_2RR). Despite the simplicity of the active site, the CO_2-to-CO mechanism on Fe-N-C remains controversial. Firstly, there is a long debate regarding the rate-determining step (RDS) of the reactions. Secondly, recent computational and experimental studies are puzzled by the fact that the CO-poisoned Fe centers still remain highly active at high potentials. Thirdly, there are ongoing challenges in elucidating the high selectivity of hydrogen evolution reaction (HER) over CO_2RR at high potentials. In this work, we introduce a novel CO_2RR mechanism on Fe-N-C, which was inspired by the dynamic of active sites in biological systems. By employing grand-canonical density functional theory and kinetic Monte-Carlo, we found that the RDS is not fixed but changes with the applied potential. We demonstrated that our proposed dual-side mechanisms could clarify the reason behind the high catalytic activity of CO-poisoned metal centers, as well as the high selectivity of HER over CO_2RR at high potential. This study provides a fundamental explanation for long-standing puzzles of an important catalyst and calls for the importance of considering the dynamic of active sites in reaction mechanisms.

Biography

Prof. Shuzhou LI received his B.Sc, M.Sc, and PhD in chemistry from Nankai University, Peking University, and University of Wisconsin, respectively. After working as a postdoc in Northwestern University, he joined in Nanyang Technological University. Currently, he is a Professor in School of Materials Science and Engineering and his research interests are theoretical and computational material science. He has been focused on (1) Heterogeneous Catalysis; (2) Artificial Intelligence for Materials Discovery; (3) Flexible Electronics.

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