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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

https://iapme.um.edu.mo/

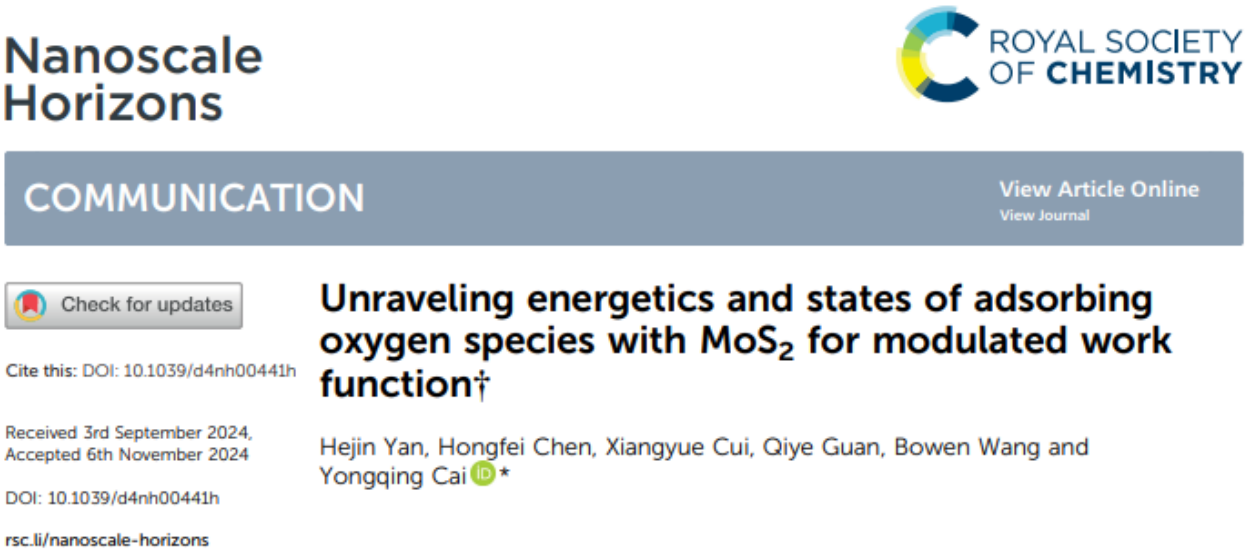
ISSUE 14

25 December 2024

✧ Content

❖ Publications (IF≥8; *corresponding author)

1. **Hejin Yan**, Hongfei Chen, Xiangyue Cui, Qiye Guan, Bowen Wang and **Yongqing Cai***. Unraveling energetics and states of adsorbing oxygen species with MoS2 for modulated work function. *Nanoscale Horizons* (2025). DOI: 10.1039/D4NH00441H. [2023 IF=8.0]



Nanoscale Horizons

ROYAL SOCIETY OF CHEMISTRY

COMMUNICATION

View Article Online
View Journal

Check for updates

Cite this: DOI: 10.1039/d4nh00441h

Received 3rd September 2024,
Accepted 6th November 2024

DOI: 10.1039/d4nh00441h

rsc.li/nanoscale-horizons

Unraveling energetics and states of adsorbing oxygen species with MoS_2 for modulated work function†

Hejin Yan, Hongfei Chen, Xiangyue Cui, Qiye Guan, Bowen Wang and Yongqing Cai *

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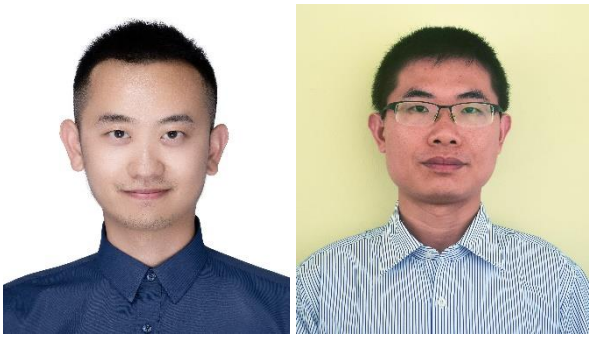
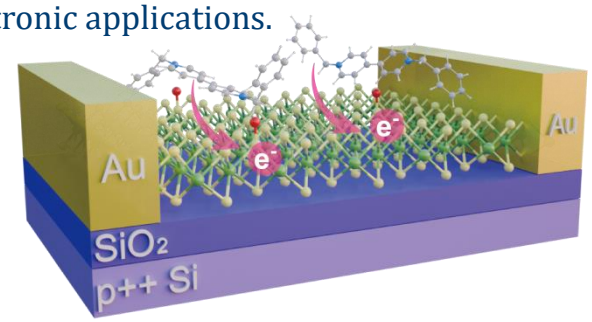
❖ Research Stories

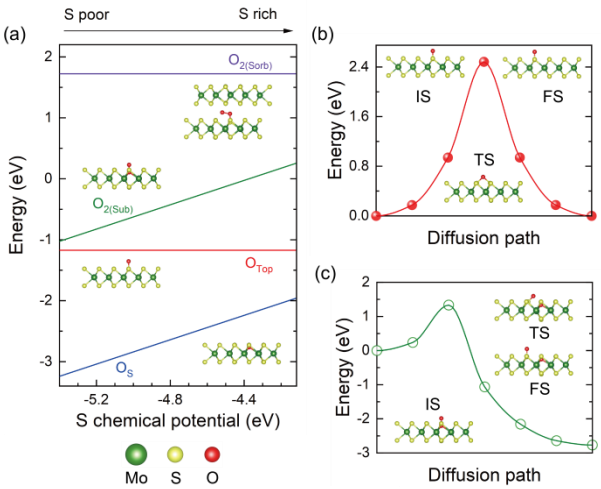
UM research team explored the oxygen absorbate modified energetics and electronic properties in MoS_2

- A promising method was reported for sulfur vacancy healing, carrier mass controlling, and contact resistance reduction in MoS_2 through oxygen dopant.
- By performing first-principles calculations, the research team identified various states of oxygen species adsorbed on the MoS_2 surface. For the first time, a "dissociative" mechanism was introduced to explain the physisorbed oxygen molecule trapped at a sulfur vacancy splitting into two chemisorbed oxygen atoms. The electron and hole masses show an asymmetric effect in response to oxygen, as a stronger hybridization of oxygen states in the valence band edge.
- Alteration of oxygen content allows modulation of the work function up to 0.5 eV, enabling reduced Schottky barriers in MoS_2/metal contact. These exciting results suggest that tuning the chemical composition of oxygen is viable for modulating the electronic properties of MoS_2 and likely other chalcogen-incorporated TMDs, which offer promise for new optoelectronic applications.



(From left)
Mr. Hejin Yan and Prof. Yongqing Cai





Studied states of oxygen species on MoS_2

Hejin Yan, Hongfei Chen, Xiangyue Cui, Qiye Guan, Bowen Wang and **Yongqing Cai** *.
Unraveling energetics and states of adsorbing oxygen species with MoS_2 for modulated work function.
Nanoscale Horizons (2025). DOI: 10.1039/D4NH00441H. [2023 IF=8.0]

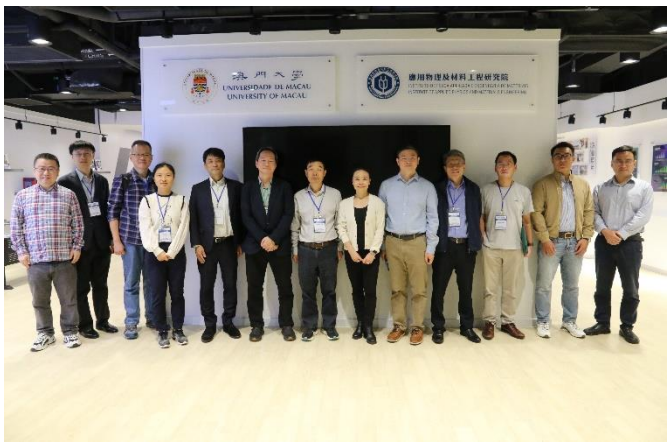
Prof. Yongqing Cai is the corresponding author of this study. The first author is Hejin Yan, a PhD. student of IAPME. This work was supported by Natural Science Foundation of Guangdong Province, China (2024A1515011161) and the Science and Technology Development Fund from Macau SAR (FDCT-0163/2019/A3, 0085/2023/ITP2, 0120/2023/RIA2). This work was performed in part at the High-Performance Computing Cluster (HPCC) which is supported by Information and Communication Technology Office (ICTO) of the University of Macau.

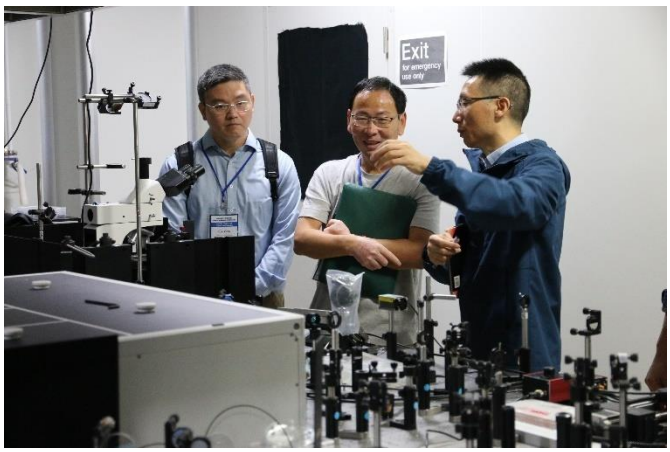
❖ UM and IAPME held the Global Academic Symposium 2024

The UM Global Academic Symposium commenced on December 2, 2024, at the University of Macau (UM). With the aim of promoting global academic exchange and strengthening international partnerships, the symposium has brought together over 50 scholars from 23 institutions across Australia, New Zealand, Singapore, South Korea, and Japan to share their research findings and advances in cutting-edge technologies, and to explore potential research collaboration.

The two-day symposium consists of four parallel sessions, one of which is the IAPME parallel session. All the participants engaged with researchers and postgraduate students in related fields through discussions, meetings, and lab tours.

The parallel session hosted by IAPME centered on “Applied Physics and Materials Engineering”, invited guests include distinguished scholars from Australia, Singapore, and Japan exchanged views with IAPME professors. Through presentations and in-depth discussions, participants explored the latest developments in nanotechnology, new materials development, optoelectronics, and new energy materials.





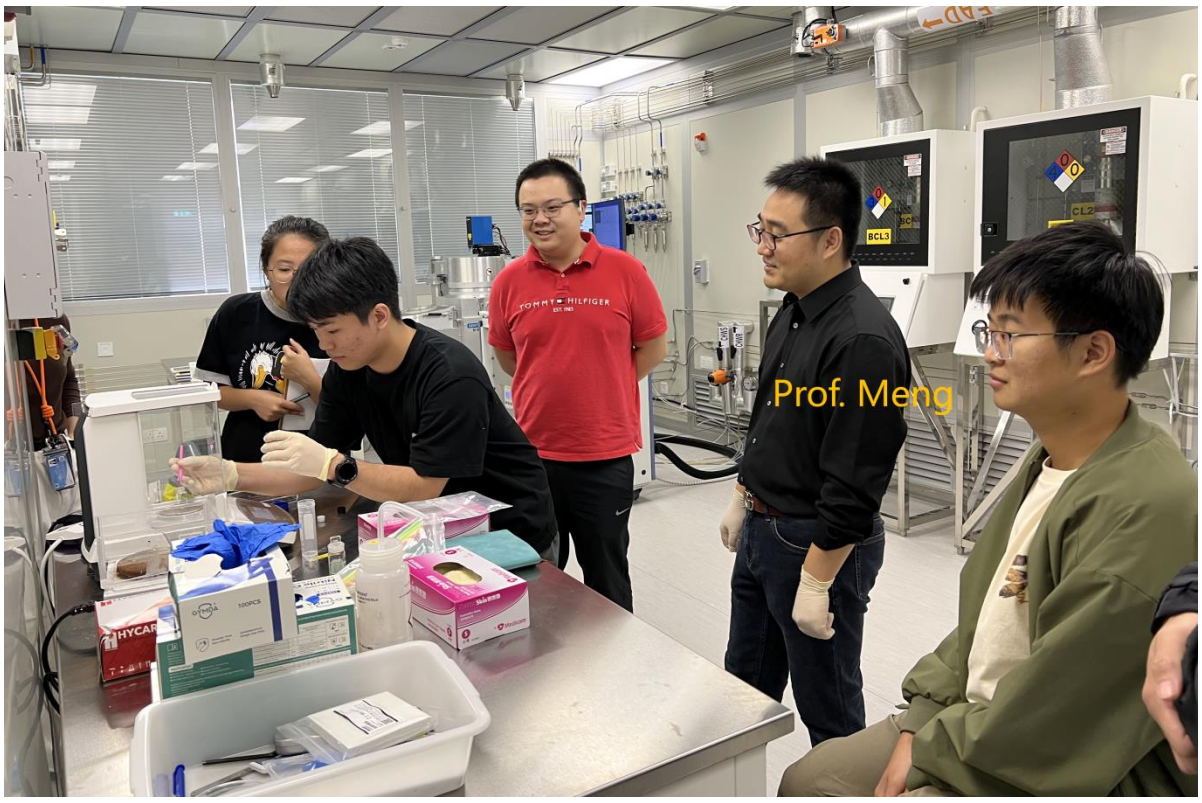
❖ Seminars

Prof. Dong Meng, Associate Professor of the School of Chemistry and Chemical Engineering at Shanghai Jiao Tong University, visited IAPME on December 6, 2024. During his visit, he delivered an insightful presentation titled "Noncovalent π-stacked Organic Framework (πOF)." The seminar was hosted by Prof. Pengzhan Sun.

Prof. Meng, who pioneered the concept of π-stacked organic frameworks, received PhD degree in the Institute of Chemistry at Chinese Academy of Sciences in 2017. From 2017 to 2023, he worked as a postdoctoral research fellow at University of California, Los Angeles (UCLA). He was awarded with National Young Overseas High-Level Talents, Shanghai Young Overseas High-Level Talents, Fellow of International Association of Advanced Materials, IAAM Young Scientist Award, Vebleo Fellow Jr. and Chinese Dean of Science Institute Award.

During his talk, Prof. Meng highlighted the significant advantages of novel porous organic molecular materials based on non-covalent interactions, particularly π-stacked organic frameworks (πOFs), over metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). πOFs form crystalline networks through π-π interactions, providing flexibility, reversibility, conductivity, solution processability, self-healing capability, high carrier mobility, and excellent stability. Based on these characteristics, Prof. Meng vividly introduces the applications of πOFs in targeted drug delivery and photocatalysis, etc., and shares the wonderful results they have achieved in their lab.

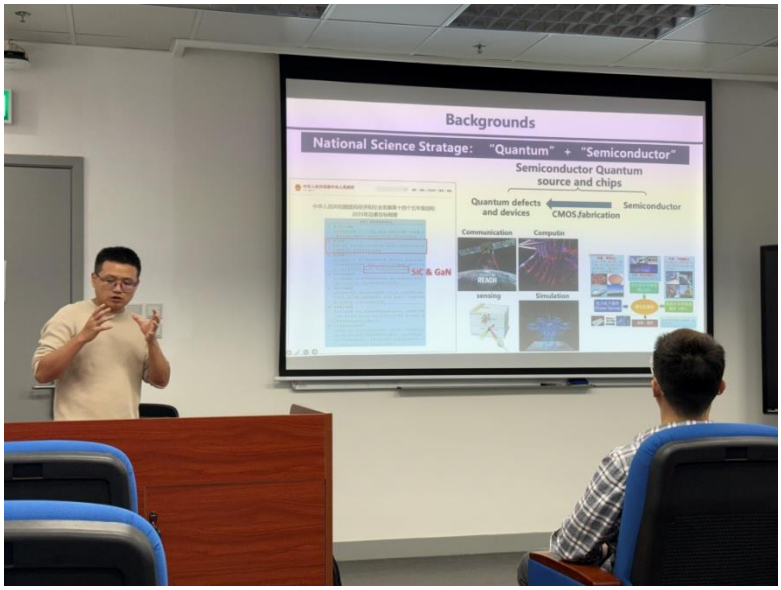
The seminar offered attendees a fresh perspective on organic porous frameworks. During the Q&A session, Prof. Meng engaged enthusiastically with the audience. Additionally, in response to students' questions, Prof. Meng entered the lab to conduct a practical demonstration for IAPME PhD students.



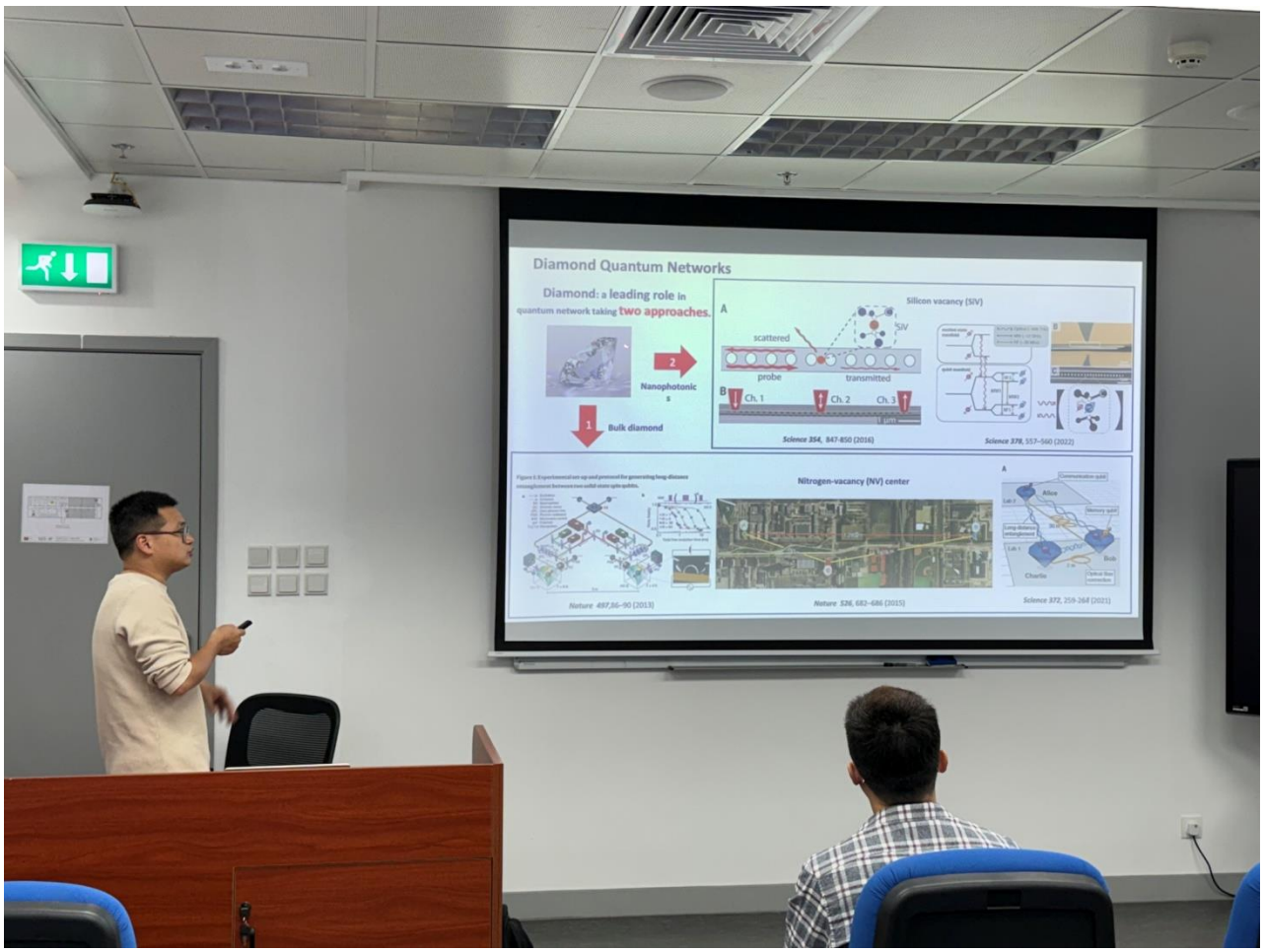
❖ Seminars

Prof. Yu Zhou, Professor of the School of Integrated circuit at the Harbin Insitute of Technology (Shenzhen), delivered an engaging talk on the "Room-Temperature Waveguide Integrated Quantum Register in a Semiconductor Photonic Platform" on 6 December 2024. Prof. Zhou shared his latest breakthroughs in the field of silicon carbide integrated photonic quantum entanglement devices, advancing the application of integrated photonic quantum information technology in quantum networks and quantum sensing.

With an impressive publication record, Prof. Zhou has authored 10 high-impact SCI papers as the first or corresponding author, including 4 in prestigious journals like Nature Communications and 1 in Science Advances. He also contributed a featured cover article in Photonics Research in 2024. He has been invited to deliver numerous talks at international conferences and workshops, showcasing his expertise in quantum defects and nano-optics. His accolades include recognition in Forbes' 30 Under 30 for his work in technology and the 9th recipient of the China Association for Science and Technology Young Talent Support. In 2024, he was honored as a committee member of the Guangdong Quantum Technology Alliance, contributing to the development of quantum technologies in China.



In his presentation, Prof. Zhou provided a comprehensive overview of recent advancements in the controlled preparation and coherent manipulation of silicon carbide (SiC) color centers on insulating substrates. He discussed the theoretical principles underpinning these techniques and their practical implementation. Prof. Zhou highlighted the successful coherent control of individual ^{13}C nuclear spins on insulating SiC substrates, achieving near-unity polarization of single nuclear spins. Additionally, he demonstrated the integration of SiC quantum registers into photonic waveguides, realizing two-qubit entanglement with a maximally entangled state fidelity of 0.89 on an integrated photonic platform. His broader research interests include the exploration of scalable quantum photonic technologies and the application of SiC-based systems in quantum networks and quantum sensing.



❖ Seminars

Dr. Tomi Pekka Bernhard Nissinen, visited IAPME on December 6, 2024. During his visit, he delivered an insightful presentation titled “Impactful Innovation -Strategic views to promote commercialization & Brief Introduction to Cementitious ternary system.” The seminar was hosted by Prof. Guoxing Sun who extended the invitation to Dr. Tomi Pekka Bernhard Nissinen.

Dr. Tomi Nissinen is a Lead Research Scientist at Kiilto Oy, a Finnish chemical and construction material manufacturer. Dr. Nissinen obtained his PhD degree of Chemistry from University of Bristol in 2014. Before his industrial experience his main research interest were in colloidal chemistry, non-classical crystallisation and biomineralization, where he has published RSC papers on gypsum crystallisation.

In his speech, he first introduced innovation models, their applications in different industries, and how companies plan their research strategies based on these models. Different tools for evaluating ideas and research topics were also presented.

The second part focused on the chemistry of aluminous cement and its application in construction materials, particularly in self-leveling substrate products.

The seminar provided attendees with a comprehensive understanding of the latest advancements in Cementitious Ternary System. Their findings contribute to the ongoing efforts to develop more eco-friendly and high-performance construction materials.

❖ Upcoming Events

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IAPME Seminar

The improvement of corrosion resistance of wet-cast concrete subjected to early-age ambient pressure carbonation curing

26 December 2024

Prof. Xiangping XIAN
City University of Hong Kong
Venue: N23-4018
Time: 11:00 - 12:00
Hosted by: Prof. Binmeng CHEN

Abstract

This presentation will mainly discuss the possibility of developing early-age ambient pressure carbonation curing to lower the corrosion risk and improve the resistance by avoiding deep CO_2 penetration and chemically and physically densifying the concrete surface layer. In addition to superior CO_2 uptake and compressive strength, the effectiveness of ambient pressure carbonation on corrosion resistance of concrete was evaluated by two methods, an accelerated impressed current method and long-term ponding methods (ASTM G109). Due to improved physical properties, carbonation-cured concrete had a lowered current reading, a reduced rebar mass loss, a lessened total or free chloride content, and a decreased chloride diffusivity. In conclusion, ambient pressure carbonation-cured concrete is corrosion resistant while still having the capacity to sequestrate carbon dioxide, which could contribute to sustainability and a circular carbon economy.

Biography

Prof. Xian is now working as an Assistant Professor in the Department of Architecture and Civil Engineering at City University of Hong Kong. He attained his master degree and Ph.D. in Civil Engineering from McGill University in 2017 and 2021 respectively. In 2023, he was also one of the Marie Sklodowska-Curie Future Roads Fellow recipients under the supervision of Prof. Abir Al-Tabbaa from Cambridge University. His research is mainly about producing green and functional cement-based products made from OPC, industrial waste (i.e., steel slag), municipal solid waste incineration (MSWI) residues, concrete waste, etc., through Carbon, Capture, Utilization, and Storage (CCUS) aiming to make contributions to both environmental protection and sustainable development. Beyond that, Prof. Xian is also interested in automation construction, 3D printing of green construction materials, the engineering application of durable materials and so on.

Enquiry: iampe.enquiry@um.edu.mo

Contact Us

Email
iapme.enquiry@um.edu.mo