

Hui PAN (潘暉)

huipan@um.edu.mo · (853) 88224427 · N23-4003, University of Macau, Taipa, Macau, China

Dr. Hui Pan is a professor and the associate director in the Institute of Applied Physics and Materials Engineering at the University of Macau. He got his PhD degree in Physics from the National University of Singapore in 2006. From 2006 to 2013, he worked at National University of Singapore as a Research Fellow, Oak Ridge National Laboratory (USA) as a Postdoctoral Fellow, and Institute of High-Performance Computing (Singapore) as a Senior Scientist, respectively. He joined the University of Macau as an assistant professor in 2013. Dr. Pan was promoted to associate professor in 2017 and full professor in 2020. In his research, a combined computational and experimental method is used to design and fabricate novel nanomaterials for applications in green energy and environments (such as electro-/photo-catalysis, water splitting, CO₂/NO₃ reduction, and green hydrogen), electronic/quantum devices, and spintronics. He has published ~ 300 papers in international peer-reviewed journals. The total citation is ~ 21,100 (google scholar). Additionally, he is the author of 5 book chapters and the inventor of 4 USA and 10 China patents. His present h-index is 81 (google scholar). (updated in Aug. 2025).

Education

- Ph.D. in Physics, National University of Singapore, Singapore (2006)
- Bachelor in Electronic Materials and Devices, Xidian University, Xi'an, China (1997)

Professional Experience

- Associate Director of the Institute of Applied Physics and Materials Engineering, University of Macau, Macau (05/2022 – Present)
- Professor, University of Macau, Macau (08/2020 – Present)
- Founding Head of Department of Physics and Chemistry, Faculty of Science and Technology, University of Macau, Macau (08/2018 – 06/2022)
- Associate Professor, University of Macau, Macau (08/2017 – 08/2020)
- Assistant Professor, University of Macau, Macau (08/2013 – 08/2017)
- Senior Scientist I, Institute of High Performance Computing, Singapore (03/2013 – 08/20213)
- Scientist II, Institute of High Performance Computing, Singapore (04/2012 – 03/2013)
- Scientist I, Institute of High Performance Computing, Singapore (05/2009 – 03/2012)
- Postdoctoral Fellow, Oak Ridge National Laboratory, USA (04/2008 – 04/2009)
- Research Fellow, National University of Singapore, Singapore (01/2006 – 03/2008)

Teaching

B.Sc. Courses

1. Solid State Physics

PhD Courses

1. Advanced Instrumentation for Materials Characterization

Research

Research Interests

- Energy harvesting and storage (photocatalysis, electrocatalysis, CO₂/NO₃ reduction, Water Splitting, hydrogen production)
- Spintronics
- Nanodevices (ReRAM and PRAM)
- Fabrication and first-principles design of materials
- Condensed Matter Physics

Research Grants

Grants from Macau/Shenzhen Government:

- Science and Technology Development Fund from Macao SAR (FDCT/0050/2023/RIB2) (from 01/2024 to 01/2027) (on-going)
- Science and Technology Development Fund from Macao SAR (FDCT/0023/2023/AFJ) (from 12/2023 to 12/2026) (on-going)
- Science and Technology Development Fund from Macao SAR (FDCT- 0111/2022/A2) (from 12/2022 to 12/2025) (on-going)
- Shenzhen-Hong Kong-Macao Science and Technology Research Programme (Type C) (SGDX20210823103803017) (from 04/2022 to 04/2024)
- Science and Technology Development Fund from Macao SAR (FDCT- 0028/2021/APD) (from 04/2022 to 03/2024)
- Science and Technology Development Fund from Macao SAR (FDCT- 0081/2019/AMJ) (from 01/2021 to 12/2023)
- Science and Technology Development Fund from Macao SAR (FDCT- 0154/2019/A3) (from 05/2020 to 05/2023)
- Science and Technology Development Fund from Macao SAR (FDCT- 0102/2019/A2) (from 08/2019 to 07/2022)
- Science and Technology Development Fund from Macao SAR (FDCT- 0035/2019/AGJ) (from 01/2020 to 12/2021)
- Science and Technology Development Fund from Macao SAR (FDCT- 110/2014/SB) (from 11/2015 to 10/2018)
- Science and Technology Development Fund from Macao SAR (FDCT-132/2014/A3) (from 06/2015 to 05/2018)
- Science and Technology Development Fund from Macao SAR (FDCT-062/2014/A) (from 01/2015 to 12/2017)
- Science and Technology Development Fund from Macao SAR (FDCT-076/2013/A) (from 01/2014 to 12/2014)

Grants from University of Macau:

- Multi-year research grant at University of Macau (MYRG-GRG2025-00007-IAPME) (from 01/2026 to 12/2027) (on-going)
- Multi-year research grant at University of Macau (MYRG-GRG2024-00038-IAPME) (from 01/2025 to 12/2026) (on-going)

- Multi-year research grant at University of Macau (MYRG-GRG2023-00010-IAPME) (from 01/2024 to 12/2025)
- Multi-year research grant at University of Macau (MYRG2022-00026-IAPME) (from 01/2023 to 12/2024)
- Multi-year research grant at University of Macau (MYRG2018-00003-IAPME) (from 01/2019 to 12/2021)
- Multi-year research grant at University of Macau (MYRG2017-00027-FST) (from 01/2018 to 12/2020)
- Multi-year research grant at University of Macau (MYRG2015-00017-FST) (from 04/2015 to 09/2018)
- Start-up research grant at University of Macau (SRG2013-00033-FST) (from 10/2013 to 09/2015)
- Multi-year research grant at University of Macau (MYRG2014-000159-FST) (from 05/2014 to 04/2017)

Research Laboratory

Catalysis and Energy Materials Laboratory: N23-2005/6

Current Members

PhD, Master and UG Students

Mr. Yatai Li (PhD student, 08/2025 ~ present)
 Mr. Botao Fan (PhD student, 08/2025 ~ present)
 Ms. Zimo Zhang (PhD student, 08/2025 ~ present)
 Mr. Zhenyu Zhang (PhD student, 08/2025 ~ present)
 Mr. Wendi Zhang (PhD student, 08/2024 ~ present)
 Mr. Chengcheng Zhong (PhD student, 08/2024 ~ present)
 Ms. Xiaoling Lai (PhD student, 08/2024 ~ present)
 Ms. Ziwen Feng (PhD student, 08/2024 ~ present)
 Ms. Juanjuan Wang (PhD student, 08/2024 ~ present)
 Mr. Jianke Tao (PhD student, 08/2023 ~ present)
 Ms. Hongling Liu (PhD student, 08/2023 ~ present)
 Ms. Jiao Yang (PhD student, 08/2023 ~ present)
 Ms. Junge Yang (PhD student, 08/2023 ~ present)
 Mr. Yiqian Chen (Undergraduate, 10/2022 ~ present)
 Mr. Zichao Yu (PhD student, 08/2022 ~ present)
 Mr. Yirui Yang (Master student, 08/2025 ~ present)
 Mr. Haoyu Wu (Master student, 08/2025 ~ present)
 Ms. Junting Chen (Master student, 08/2025 ~ present)
 Mr. Wuri Bao (Master student, 08/2024 ~ present)
 Mr. Xingyou Li (Master student, 08/2024 ~ present)
 Mr. Yuzhe Shen (Master student, 08/2024 ~ present)
 Mr. Iek Him Chen (Undergraduate, 10/2022 ~ present)
 Ms. Ka Ka Ng (Undergraduate, 06/2024 ~ present)
 Ms. Si Ham Li (Undergraduate, 06/2024 ~ present)
 Mr. Yueyang Wu (Undergraduate, 05/2024 ~ present)
 Mr. Xiaoni Qiu (Undergraduate, 10/2025 ~ present)
 Ms. Pinxuan Liu (Undergraduate, 10/2025 ~ present)

Research Staff:

Mr. Lun LI
Mr. Youpeng CAO
Dr. Di LIU
Dr. Jinxian FENG
Dr. Yuxuan XIAO
Dr. Jingxia QIAN

Former Members***PhD Graduates***

Dr. Yuanju Qu, Roger (PhD study from 08/2014 ~ 08/2017)
Dr. Ziqian Ma, Mason (PhD study from 08/2014 ~ 04/2018)
Dr. Mengmeng Shao (PhD study from 08/2016 ~ 06/2019)
Dr. Wenzhou Chen (PhD study from 08/2016 ~ 06/2019)
Dr. Xiongwei Zhong (PhD study from 08/2016 ~ 10/2019)
Dr. Lujie Cao (PhD study from 01/2016 ~ 01/2020)
Dr. Mingyang Yang (PhD study from 01/2016 ~ 01/2020)
Dr. Qing Zhu (PhD study from 08/2017 ~ 07/2020)
Dr. Yangfan Shao (PhD study from 08/2016 ~ 07/2020)
Dr. Rui Tong (PhD study from 08/2017 ~ 08/2020)
Dr. Dong Liu (PhD study from 01/2019 ~ 08/2021)
Dr. Youchao Kong (PhD study from 08/2018 ~ 08/2021)
Dr. Zhiqin Ying (PhD study from 08/2018 ~ 10/2021)
Dr. Chon Chio Leong, Roy (PhD study from 08/2014 ~ 12/2021)
Dr. Xinyu Du (PhD study from 08/2019 ~ 06/2022)
Dr. Haoqiang Ai (PhD study from 08/2019 ~ 06/2022)
Dr. Jiazhong Geng (PhD study from 08/2019 ~ 06/2022)
Dr. Feifei Li (PhD study from 08/2019 ~ 06/2022)
Dr. Mingpeng Chen (PhD study from 08/2019 ~ 06/2022)
Dr. Kin Long Ao (PhD study from 08/ 2017 ~ 10/2022)
Dr. Di Liu (PhD study 08/2020 ~ 07/2023)
Dr. Jinxian Feng (PhD study 08/2020 ~ 07/2023)
Dr. Bowen Li (PhD study 08/2019 ~ 07/2023)
Dr. Pengfei Zhou (PhD study 08/2019 ~ 07/2023)
Dr. Haoyun Bai (PhD study, 08/2020 ~ 07/2024)
Dr. Lulu Qiao (PhD study, 08/2021 ~ 08/2024)
Dr. Chunfa Liu (PhD study, 08/2022 ~ 06/2025)
Dr. Shuyang Peng (PhD study, 08/2022 ~ 06/2025)
Dr. Yutong Li (PhD study, 08/2022 ~ 06/2025)
Dr. Lihong Yin (PhD study, 08/2021 ~ 10/2025)
Dr. Zhongheng Li (PhD study, 08/2021 ~ 12/2025)

Master graduates

Mr. Yanhong Liu (Master, 08/2023 ~ 06/2025)

Undergraduates

Mr. Shijie Wen, Jack (graduated in 2016)
Mr. Yifeng Xie (graduated in 2018)
Mr. Jialin Li (graduated in 2018)

Mr. Ye Ke (graduated in 2018)
Mr. Jer Shiuh Phooh (graduated in 2019)
Ms. Ziqin Dai, Helen (graduated in 2019)
Mr. Shengjie Ding (graduated in 2020)
Mr. Yunxiao Liu (graduated in 2023)
Mr. Xuanwei Dai (graduated in 2024)
Mr. Jiachen Li (graduated in 2025)
Mr. Li-Hung Yao (graduated in 2025)

Research Staff

Mr. Di Liu (currently Postdoctoral fellow in my Group)
Dr. Zhen Li (@Shandong Normal University, Shandong, China)
Dr. Chi Fong Wong (@City Univerisyt of Macau, Macao SAR)
Dr. Tianwei He (@ Fritz Haber Institute of the Max Plank Society Berlin, Germany)
Dr. Pengcheng Zhao (@Northeast Petroleum University)
Dr. Chao Peng (@WuYi University, Jiangmen, Guangdong, China)
Dr. Zhongbing Pan (@ Lingbo University, Lingbo, Zhejiang, China)
Dr. Xuejian Du (@Shandong Normal University, Shandong, China)
Dr. Roger Yuanju QU (@Linkoping University, Sweden)
Mr. Wenhao Gu (@Macau University of Science and Technology (Macao SAR))
Dr. Qingchun ZHANG (@Southwest University of Science and Technology)
Mr. Chunfa LIU (currently PhD student in my Group)
Dr. Yuyun CHEN (@ Guangxi Nationality University)
Dr. Siying SHEN
Dr. Songbo CHEN (@ Shenzhen University)
Dr. Yuling ZHOU (@ Shenzhen University)
Dr. Yuzhe LIU (@ Shenzhen University)
Dr. Shangpeng LI (@ Shenzhen University)
Dr. Lianyi SHAO (@ Guangdong University of Technology)
Dr. Xingshuai LYV (@ Ocean University of China)
Dr. Katherine Weng I CHIO
Mr. Yatai LI (Currently PhD student in my group)
Mr. Zhenyu ZHANG (Currently PhD student in my group)

Links

<https://iapme.um.edu.mo/people/academic-staff/pan-hui/>
<https://www.fst.um.edu.mo/pc/acadstaff.html>
<https://publons.com/researcher/2877040/hui-pan/>
<http://scholar.google.com.sg/citations?user=vmGv38sAAAAJ&hl=en>
<https://orcid.org/0000-0002-6515-4970>
<https://www.scopus.com/authid/detail.uri?authorId=57192713115>

Patent List:

1. **Hui Pan** and Di Liu, General preparation method for noble metal-supported TM hydroxides for electrocatalytic nitrate reduction reaction to produce ammonia. **China Patent Application**,
2. **Hui Pan** and Yuxuan Xiao, A method for synthesis of structurally reversible Bi-based catalyst and its application in electrochemical CO₂ reduction reaction. **China Patent Application No. "202510113710.3"**.
3. **Hui Pan** and Jingxian Feng, A high-efficient and low-cost Sn-Zn alloy based electrocatalyst for CO₂-to-formate electrochemical reduction. **China Patent Application No. "202510371543.2"**
4. **Hui Pan** and Youpeng Cao, Preparation and application of supra-nanometer-sized ruthenium-platinum alloy catalyst. **China Patent Application No. "202411512854.8"**
5. **Hui Pan** and Youpeng Cao, Preparation and application of ruthenium-platinum sub-nanometer alloy catalyst. **China Patent Application No. "202410819532.1"**
6. **Hui Pan** and Jingxian Feng, A high efficient copper based electrocatalyst for CO₂-to-ethylene electrochemical reduction. **China Patent Application No. "202411185483.7"**
7. **Hui Pan** and Wenhao Gu, Copper-manganese co-incorporated titanium-based metal-organic framework photocatalyst for efficient reduction of carbon dioxide to formic acid. **China Patent Application No. "202410432503.X"**.
8. **Hui Pan** and Yuxuan Xiao, An in-situ construction method for synthesis of flower-like bismuth trioxide/bismuth subcarbonate heterojunction and its application in electrochemical CO₂ reduction reaction. **China Patent Application No. "202410515435.3"**.
9. **Hui Pan** and Lun Li, A simple, inexpensive and efficient method for synthesizing γ -FeOOH for OER reaction. **China Patent Application No. "202510372525.6"**.
10. **Hui Pan**, Chunfa Liu, and Hongchao Liu, A method for preparing an efficient and stable iron-based oxygen evolution electrocatalyst for industrial water electrolysis. **China Patent Application No. "202411711710.5"**.
11. **Hui Pan** and Lun Li, Preparation method and application of a high entropy electrocatalyst. **China Patent Application No. "202410468967.6"**.
12. **Hui Pan**, Chunfa Liu, Hongchao Liu, and Shuangpeng Wang, A facile method for the preparation of low-cost, efficient and stable transition metal-based OER electrocatalysts. **China Patent Application No. "202410146052.3"**.
13. **Hui Pan** and Jinxing Feng, Low-cost and high-performance electrocatalyst based on surface Sn incorporation brass for CO₂-to-formate electrochemical reduction, **China Patent Application No. "202311383783.1"**.
14. **Hui Pan**, Chunfa Liu, and Hongchao Liu, Bi-functional and low-cost electrocatalyst for high-efficient and stable full-water-splitting: FeCoCrCuOx@CF, **China Patent Application No. "202310523696.5"**.
15. **Hui Pan**, Shuyang Peng, and Kin Ho Lo, Low Cost, High Efficiency and Stability Industrial Si-based Photoelectrochemical Materials for Water Splitting, 11/07/2023, **China Patent Application No. "202311350080.9"**.
16. **Hui Pan**, Rucheng Wu, and Di Liu, A simple way to make Si-based photoelectrode with active layer for Solar-driven water splitting with high Saturation Photocurrent. 31/10/2022, **Granted, China Patent No. "ZL202211344350.0"**.
17. **Hui Pan**, Di Liu, Shuangpeng Wang, Lulu Qiao, and Kar-Wei Ng, Low-cost electrocatalyst for high-efficient and stable nitrate reduction reaction. **Granted, China Patent No. "ZL202210554712.2"**.

18. **Hui Pan**, Pengfei Zhou, Shuangpeng Wang, and Kar-Wei Ng, Bi-functional and low-cost electrocatalyst for high-efficient and stable full-water-splitting: stainless steel treated by simple anodization in saline. 16/06/2021, **Granted, China Patent No. “202110856193.0”**.
19. **Hui Pan**, Dong Liu and Guichuang Xing, “Bi-functional and low-cost electrocatalyst for high-efficient and stable full-water-splitting: Cr-doped NiS_x”, 13/12/2022, **Granted, China Patent No. “ZL201910758027. X”**.
20. **Hui Pan** and Mengmeng Shao, “MoS₂/Mo₂C/CdS: a super-efficient photocatalyst for hydrogen evolution”, 30/08/2020, **Granted, China Patent No. “ZL201811323293.1”**.
21. **Hui Pan** and Xiongwei Zhong, “Carbon-Coated N-rich C₃N₄ as an anode material for Lithium Battery”, 12/02/2018, **Granted, China Patent No. ZL 201810148357.2**.
22. **Hui Pan** and Yuanju Qu, “TiS₂: an excellent cathodic electrocatalyst for hydrogen production in electrolysis of water”, 26/09/2017, **Granted. China Patent No. ZL 201710917164.4**.
23. Soo Jin Chua, Hailong Zhou, Jianyi Lin, **Hui Pan**, “Method of ZnO Film Grown on the Epitaxial Lateral Overgrowth GaN Template”, 04/25/2006, **US Provisional Patent Application No. 60/794,775**.
24. **Hui Pan**, Jianyi Lin, Yuan Ping Feng, “Supercapacitor from Carbon Tubes-in-Tube Nanostructures”, 03/01/2006, **US Provisional Patent Application No. 60/777,547**.
25. **Hui Pan**, Jianyi Lin, Yuan Ping Feng, “Synthesis of Mg doped ZnO Nanowires and Their Applications to Optical Devices and Hydrogen Storage”, 07/13/2005, **US Provisional Patent Application No. 60/698,476**.
26. **Hui Pan**, Jianyi Lin, Jun Ding, Yuan Ping Feng, “Single Crystal Growth of Magnetic Nanowires”, 11/02/2004, **US Provisional Patent Application No. 60/607,111**.

Published/Accepted journal papers (*Corresponding Author):

1. Yuxuan Xiao, Xiaoling Lai, Jinxian Feng, Ziwen Feng, Wendi Zhang, Lun Li, Weng Fai Ip*, and **Hui Pan***, Self-refreshing Bi-based active sites for efficient and durable electrochemical CO₂ reduction. *Adv. Func. Mater.* **e23592** (2026).
2. Juanjuan Wang, Yuxuan Xiao, Jinxian Feng, Chunfa Liu, Lun Li, Youpeng Cao, Chengcheng Zhong, Ziwen Feng, Wendi Zhang, Zhi-Quan Liu* and **Hui Pan***, Phosphorus incorporation in cobalt molybdate: Controlling Mo leaching for surface reconstruction to improve hydrogen evolution. *Chem Eng. J* **525**, 170812 (2025).
3. Zhongheng Li, Zheng Shu, Lun Li, Wendi Zhang, Jiaqian Kang, Chengcheng Zhong, Ziwen Feng, Jinxian Feng*, Hou Ian* and **Hui Pan***, Identifying Beneficial and Adverse Co⁴⁺ Species in Cobalt-Based Oxygen Evolution Catalysts via Precursor Polymorphism Engineering. *Adv. Sci.* **12**, e09145 (2025).
4. Wendi Zhang, Yuxuan Xiao, Lun Li, Zhichao Yu, Jinxian Feng, Chengcheng Zhong, Weng Fai Ip, and **Hui Pan***. Dynamic Mo leaching and vacancy engineering synergize HER and OER kinetics in NiFe-based catalysts for overall water electrolysis. *Mater. Horiz.* **12**, 10901 - 10910 (2025).
5. Jiarui Lin, Lianyi Shao*, Shige Wang, Shilin Zhou, Lu Yu, Xiaoyan Shi, Junling Xu, Zhipeng Sun* and **Hui Pan***, Nitrogen-doped carbon-modified Fe₃Se₄ as high pseudocapacitive anode for fast sodium-ion storage. *J. Energy Storage* **139**, 118818 (2025).
6. Hongling Liu, Zhichao Yu, Jia Zhao, Weng Fai Ip*, Sen Lin, and **Hui Pan***, Electrochemical CO₂ Reduction on Janus Dual-Atom Catalysts: Critical Role of Oxygen Coordination and an Effective Descriptor. *Adv. Sci.* **12**, e07849 (2025).
7. Yuanguo Chen, Haoyun Bai, Jiao Lan, Cheng-Wei Kao, Feng Xie, Linghu Meng, Jilong Li, Ying-Rui Lu, Ming Peng, **Hui Pan** and Yongwen Tan*, Ru single atoms anchored in metal borides enable hydrogen spillover for superior electrochemical ammonia production. *Angew. Chem. Int. Ed.* **64**, e202504568 (2025).
8. Xiaoling Lai, Jinxian Feng, Yuxuan Xiao, Weng Fai Ip*, and **Hui Pan***. Perspective on electrochemical CO₂ reduction in CO₂/O₂ mixed gas, *RSC Sust.* **3**, 4426-4434 (2025).
9. Youpeng Cao, Hongling Liu, Yuxuan Xiao, Lun Li, Jiao Yang, Chunfa Liu, Chengcheng Zhong, Wendi Zhang, Shuyang Peng, Junge Yang, Zhichao Yu, Weng Fai Ip, and **Hui Pan***, Oxygen-modified supra-nanometer-sized RuPt for robust alkaline HER/HOR. *J. Mater. Chem. A* **13**, 20838-20849 (2025).
10. Shuyang Peng, Di Liu, Zhiqin Ying, Keyu An, Chunfa Liu, Weng Fai Ip, Kin Ho Lo*, and **Hui Pan***, Bridge Layer-Enabled Silicon-Based Photoanode With High Photocurrent Density for Efficient and Stable Water Splitting. *Carbon Energy* **7**, e70052 (2025).
11. Jiaqian Kang, Yuxuan Xiao, Lun Li, Lulu Qiao, Chunfa Liu, Chengcheng Zhong, Pengzhan Sun*, Di Liu*, Weng Fai Ip, and **Hui Pan***, Ternary Synergy in Layered Double Hydroxides for Efficient and Stable Nitrate Reduction. *Adv. Func. Mater.*, 2507619 (2025).
12. Yuxuan Xiao, Di Liu, Jiao Yang, Jinxian Feng, Wenhao Gu, Lulu Qiao, Weng Fai Ip, and **Hui Pan***, Controllable Reconstruction of β -Bi₂O₃/Bi₂O₂CO₃ Composite for Highly Efficient and Durable Electrochemical CO₂ Conversion. *Nano Lett.* **25**, 6548 - 6555 (2025).
13. Zhichao Yu, Lun Li, Keyu An, Hongling Liu, Xingshuai Lv, Weng Fai Ip, and **Hui Pan***, Inverted Trends of the Brønsted - Evans - Polanyi Relation in N₂ Dissociation Originated from a Bonding-Dependent Adsorption Mechanism. *ACS Appl. Mater. Interf.* **17**, 26491-26500 (2025).
14. Youpeng Cao, Xingshuai Lv, Jiao Yang, Keyu An, Chunfa Liu, Lulu Qiao, Zhichao Yu, Lun Li, and **Hui Pan***, Oxygen-modified Ru for efficient alkaline hydrogen evolution reaction. *Dalton Transactions* **54**, 9761-9769 (2025).

15. Haoyun Bai, Junxian Liu, Di Liu, Shuyang Peng, Hongling Liu, Kin Ho Lo, **Hui Pan***, and Liangzhi Kou*, Role of magnetic exchange in catalytic spin effects: insights from nitrite reduction on Co_3O_4 . *J. Mater. Chem. A* **13**, 15067-15074 (2025).
16. Lihong Yin, Jinxian Feng*, Weng Fai Ip*, Guangfu Luo*, and **Hui Pan***, Theoretical Insights into the Activation and Conversion of Electrochemical CO_2 Reduction on 3d Transition Metal-Doped Cu(111) Stepped Structures. *ChemElectroChem* **12**, e202500095 (2025).
17. Hongling Liu, Di Liu, Zhichao Yu, Haoyun Bai, and **Hui Pan***, Electrochemical reduction of CO_2 on pure and doped Cu_2O (111). *J. Col. Inter. Sci.* **683**, 170–177 (2025).
18. Chunfa Liu, Haoyun Bai, Jinxian Feng, Keyu An, Lun Li, Zhichao Yu, Lulu Qiao, Di Liu, Shuyang Peng, Hongchao Liu*, and **Hui Pan***, Electrodeposited Ternary Metal (Oxy)hydroxide Achieves Highly Efficient Alkaline Water Electrolysis over 1000 hours under Industrial Conditions. *Carbon Energy* **7**, e684 (2025).
19. Wenhao Gu, Jinxian Feng, Xingshuai Lv, Weng Fai Ip, and **Hui Pan***, Highly enhanced photocatalytic performance for CO_2 reduction on $\text{NH}_2\text{-MIL-125(Ti)}$: The impact of (Cu, Mn) co-incorporation. *Separation and Purification Technology* **359**, 130323 (2025).
20. Shuyang Peng, Di Liu, Haoyun Bai, Chunfa Liu, Jinxian Feng, Keyu An, Lulu Qiao, Kin Ho Lo*, and **Hui Pan***, Progress on Si-based photoelectrodes for industrial production of green hydrogen by solar-driven water splitting. *EcoEnergy* (2025). (invited review)
21. Lun Li, Lulu Qiao, Di Liu, Zhichao Yu, Keyu An, Jiao Yang, Chunfa Liu, Youpeng Cao, and **Hui Pan***, High-Valence Metals Accelerate the Reaction Kinetics for Boosting Water Oxidation. *Small* **21**, 2570040 (2025). (Front Cover)
22. Chengcheng Zhong, Yuxuan Xiao*, Jinxian Feng, Chunfa Liu, Lun Li, Weng Fai Ip, Shuangpeng Wang*, and **Hui Pan***, Revealing the hydrogen bond network effect at the electrode–electrolyte interface during the hydrogen evolution reaction. *J. Mater. Chem. A* **13**, 9049-9054 (2025).
23. Yixin Chen, Jun Meng, Miao Xu, Lulu Qiao, Di Liu, Youchao Kong, Xiaosai Hu, Qingju Liu, Mingpeng Chen, Siliu Lyu*, Rui Tong*, and **Hui Pan***, Adaptive Active Site Turning for Superior OER and UOR on Ir- Ni_3N Catalyst. *Adv. Fun. Mater.* **35**, 2413474 (2025).
24. Lebin Cai, Haoyun Bai, Jilong Li, Feng Xie, Kang Jiang, Ying-Rui Lu, **Hui Pan**, and Yongwen Tan*, Single-atom tungsten doping induced chemical–electrochemical coupled pathway on Ni(OH)₂ enables efficient urea electrooxidation. *Energy Environ. Sci.* **18**, 2415-2425 (2025).
25. Mengmeng Shao, Shushu Fu, Shiji Hao, Min Chen, Jutao Jin, Wenlong Wang, Xiaochang Qiao, Dexing Zhang, Yangfan Shao*, **Hui Pan***, and Xiaoji Wang*, Enhanced Photocatalytic H_2 Evolution with Accelerating Surface Reaction via Ru-Doped NiFe Hydroxide as Cocatalyst. *ChemCatChem* **17**, e202400827 (2025).
26. Jiangke Tao, Di Liu, Zhichao Yu, and **Hui Pan***, Enhanced reduction of CO to C2 products on MoS_2 nanoribbon by edge engineering. *J. Mater. Chem. A* **12**, 32154-32163 (2024).
27. Jinxian Feng, Xuesen Wang, and **Hui Pan***, In-situ reconstruction of catalyst in electrocatalysis. *Adv. Mater.* **36**, 2411688 (2024).
28. Lulu Qiao, Anquan Zhu, Di Liu*, Keyu An, Jinxian Feng, Chunfa Liu, Kar Wei Ng*, and **Hui Pan***, In Situ Reconstructed Cu/ β -Co(OH)₂ Tandem Catalyst for Enhanced Nitrate Electroreduction to Ammonia in Ampere-Level. *Adv. Energy Mater.* **14**, 2402805 (2024). (Front Cover)
29. Jiao Yang, Keyu An, Zhichao Yu, Lulu Qiao, Youpeng Cao, Yujuan Zhuang, Chunfa Liu, Lun Li, Lishan Peng* and **Hui Pan***, Effect of Cation and Anion Vacancies in Ruthenium Oxide on the Activity and Stability of Acidic Oxygen Evolution. *ACS Catal.* **14**, 17739-17747 (2024).
30. Jinxian Feng, Chunfa Liu, Lulu Qiao, Keyu An, Sen Lin, Weng Fai Ip, and **Hui Pan***, Electrolyte-Assisted Structure Reconstruction Optimization of Sn-Zn Hybrid Oxide Boosts the Electrochemical CO_2 -to- HCOO^- Conversion. *Adv. Sci.* **11**, 2407019 (2024).

31. Junge Yang, Jinxian Feng, Youpeng Cao, Yuxuan Xiao, Lulu Qiao, Keyu An, Jiao Yang, Jing Peng*, **Hui Pan***, and Hui-Ming Cheng*, Highly Dispersed Ru-Pt Heterogeneous Nanoparticles on Reduced Graphene Oxide for Efficient pH-Universal Hydrogen Evolution. *Adv. Fun. Mater.* **34**, 2411081 (2024).
32. Hong Lin, Zhiliang Guo, Qingchun Zhang*, Qin Yang, Meng Wang, Yuanyuan Chen, Shiyang Shen, Xijun Wei, Lixian Song, Yingze Song*, and Hui Pan*, Coupled Ni–Co Dual-Atom Catalyst for Guiding Sulfur and Lithium Evolutions in Lithium–Sulfur Batteries. *Small* **14**, 2404983 (2024).
33. Shuyang Peng, Di Liu, Zhiqin Ying, Keyu An, Chunfa Liu, Jinxian Feng, Haoyun Bai, Kin Ho Lo*, and **Hui Pan***, Industrial-Si-based photoanode for highly efficient and stable water splitting. *J. Col. Inter. Sci.* **671**, 434-440 (2024).
34. Dong Liu*, Yaohai Cai, Xin Wang, Yuling Zhuo, **Hui Pan***, and Zhenbo Wang*, Innovations in Electrocatalysts, Hybrid Anodic Oxidation, Electrolyzers for Enhanced Direct Seawater Electrolysis. *Energy Environ. Sci.* **17**, 6897-6942 (2024).
35. Mingpeng Chen*, Huachuan Sun, Qingjie Lu, Dequan Li, Di Liu, Tong Zhou, Baoye Zi, Hongshun Zheng, Bin Xiao, Tianwei He, Jianhong Zhao, Yumin Zhang, Jin Zhang, Feng Liu, Hao Cui, **Hui Pan***, and Qingju Liu*, Shining light on atomic vacancies in electrocatalysts for boosted water splitting. *Chem. Eng. J* **497**, 154235 (2024).
36. Shanpeng Li, Yuling Zhuo, Dong Liu*, **Hui Pan***, and Zhenbo Wang*, Anchoring highly surface-exposed Pt single atoms on Ni₃S₂/Co₉S₈ with abundant S vacancies triggers d-orbital electron rearrangements for boosted seawater hydrogen evolution. *Appl. Catal. B* **355**, 124188 (2024).
37. Keyu An, Zhichao Yu, Haoyun Bai, Di Liu, Lulu Qiao, Xingshuai Lv, Lianyi Shao, Jinxian Feng, Youpeng Cao, Lun Li, Zhaorui Wen, Shi Chen, Zhongbin Pan, Shuangpeng Wang*, and **Hui Pan***, Oxygen vacancy redistribution and ferroelectric polarization relaxation on epitaxial perovskite films during an electrocatalytic process. *J. Mater. Chem. A* **12**, 9672-9680 (2024).
38. Di Liu, Shuyang Peng, Lulu Qiao, Haoyun Bai, Keyu An, Chunfa Liu, Mingpeng Chen, Kin Ho Lo, Kar Wei Ng, Shengjie Peng, Shuangpeng Wang*, Weng Fai Ip*, and **Hui Pan***, Rational Design of Cocatalyst for Highly Improved Ammonia Production from Photoelectrochemical Nitrate Reduction. *Appl. Catal. B*, **351**, 123980 (2024).
39. Songbo Chen, Yuling Zhuo, Xin Wang, Shanpeng Li, Jianxi Lu, Dong Liu*, **Hui Pan***, and Zhenbo Wang*, Advances of layered double hydroxide electrocatalysts for high-current-density alkaline water/seawater splitting. *Coordination Chem. Rev.* **510**, 215832 (2024).
40. Haoyun Bai, Weng Fai Ip, Wenlin Feng, and **Hui Pan***, Effect of ferroelectric polarization on oxygen evolution reaction: a theoretical study of M₂IrSn₂S₆ (M= Bi, Mn, and Sb). *J. Mater. Chem. A* **12**, 7724-7731 (2024).
41. Yutong Li, Haoyun Bai, Zhichao Yu, Chi Tat Kwok*, and **Hui Pan***, Multiferroicity in 2D MSX₂ (M= Nb and Zr; X= Cl, Br, and I). *J. Mater. Chem. C* **12**, 6131-6139 (2024).
42. Haiyang Liu, Xiaolu Liu, Chengqun Xu*, Dongyu Wang, Dezhi Li, Jingyao Huang, Shengquan Wu, Zhichun Wang, and **Hui Pan***, Molecular engineering of polymeric carbon nitride for photocatalytic hydrogen production with ultrahigh apparent quantum efficiency. *J. Mater. Chem. A* **12**, 9200 - 9211 (2024).
43. Mengmeng Shao*, Yangfan Shao, and **Hui Pan***, Progress on enhancing the charge separation efficiency of carbon nitride for robust photocatalytic H₂ production. *Phys. Chem. Chem. Phys.* **26**, 11243-11262 (2024).
44. Lebin Cai, Haoyun Bai, Cheng-wei Kao, Kang Jiang, **Hui Pan**, Ying-Rui Lu*, and Yongwen Tan*, Platinum–Ruthenium Dual-Atomic Sites Dispersed in Nanoporous Ni_{0.85}Se Enabling Ampere-Level Current Density Hydrogen Production. *Small* **20**, 2311178 (2024).

45. Zhichao Yu, Haoyun Bai, Bowen Li, Lun Li, and **Hui Pan***, Two-Dimensional Asymmetric Multiferroics: Unique Way toward Strong Magnetoelectric Coupling and Multistate Memory. *J. Phys. Chem. Lett.* **15**, 1795-1801 (2024).
46. Haoyun Bai, Zhichao Yu, Jinxian Feng, Di Liu, Weiqi Li, and **Hui Pan***, Co_3X_8 (X= Cl and Br): multiple phases and magnetic properties in Kagome lattice. *Nanoscale* **16**, 1362-1370 (2024).
47. Shuyang Peng, Di Liu, Keyu An, Zhiqin Ying, Mingpeng Chen, Jinxian Feng, Kin Ho Lo*, and **Hui Pan***, n-Si/SiO_x/CoO_x-Mo Photoanode for Efficient Photoelectrochemical Water Oxidation. *Small* **20**, 2304376 (2024).
48. Jinxian Feng, Lulu Qiao, Chunfa Liu, Pengfei Zhou, Wenlin Feng, and **Hui Pan***, Triggering efficient reconstructions of Co/Fe dual-metal incorporated Ni hydroxide by phosphate additives for electrochemical hydrogen and oxygen evolutions. *J. Col. Inter. Sci.* **657**, 705-715 (2024).
49. Lulu Qiao, Di Liu, Anquan Zhu, Jinxian Feng, Pengfei Zhou, Chunfa Liu, Kar Wei Ng*, and **Hui Pan***, Nickel-facilitated In-situ Surface Reconstruction on Spinel Co_3O_4 for Enhanced Electrochemical Nitrate Reduction to Ammonia. *Appl. Catal. B* **340**, 123219 (2024).
50. Chunfa Liu, Jinxian Feng, Pengfei Zhou, Dong Liu, Lulu Qiao, Di Liu, Youpeng Cao, Shi-Chen Su, Hongchao Liu*, and **Hui Pan***, Multi-metal interaction boosts reconstructed FeCoCrCuO_x @CF toward efficient alkaline water electrolysis under large current density. *Chem. Eng. J.* **476**, 146710 (2023).
51. Haoyun Bai, Di Liu, and **Hui Pan***, LaOMS_2 (M= Ti, V, and Cr): novel crystal spin valves without contact. *Mater. Horizon* **10**, 5126-5132 (2023).
52. Qingchun Zhang, Di Liu, Yaping Zhang, Zhiliang Guo*, Minpeng Chen, Yuyun Chen, Bo Jin, Yingze Song*, and **Hui Pan***, Insight into coupled Ni-Co dual-metal atom catalysts for efficient synergistic electrochemical CO_2 reduction. *J. Energy Chem* **87**, 509-517 (2023).
53. Zhichao Yu, Bowen Li, Haoyun Bai, and **Hui Pan***, Two-dimensional Janus perovskite oxynitrides as active photocatalysts for overall water splitting with ferroelectric modulation. *J. Chem. Mater. A* **11**, 19074-19082 (2023).
54. Xingshuai Lv, Junxian Liu, Liangzhi Kou*, Kar Wei Ng*, Shuangpeng Wang*, Thomas Frauenheim*, and **Hui Pan***, Three-Dimensional Dual-Site Catalysts for Industrial Ammonia Synthesis at Dramatically Decreased Temperatures and Pressures. *ACS Catal.* **13**, 13561-13568 (2023).
55. Lihong Yin, Zhiqiang Li, Jinxian Feng, Pengfei Zhou, Lulu Qiao, Di Liu, Zhibin Yi, Weng Fai Ip*, Guangfu Luo*, and **Hui Pan***, Facile and Stable CuInO_2 Nanoparticles for Efficient Electrochemical CO_2 Reduction. *ACS Appl. Mater. Inter.* **15**, 47135–47144 (2023).
56. Yuling Zhuo, Dong Liu*, Lulu Qiao, Songbo Chen, Jianxi Lu, Weng Fai Ip*, **Hui Pan***, and Zhenbo Wang*, Ultrafast Room-Temperature Synthesis of Large-Scale, Low-Cost, and Highly Active Ni–Fe Based Electrodes toward Industrialized Seawater Oxidation. *Adv. Energy Mater.* **13**, 2301921 (2023).
57. Shiyang Shen, Haoqiang Ai, Yandong Ma, Haoyun Bai, Xuejian Du, Feifei Li, and **Hui Pan***, In-Plane Ferroelectric Monolayer TiNbX_4O and Its Application in Bulk Photovoltaic Effect. *Appl. Phys. Lett.* **123**, 052901 (2023).
58. Songbo Chen, Dong Liu*, Pengfei Zhou, Lulu Qiao, Keyu An, Yuling Zhuo, Jianxi Lu, Qizhen Liu, Weng Fai Ip*, Zhenbo Wang*, and **Hui Pan***, Multi-metal electrocatalyst with crystalline/amorphous structure for enhanced alkaline water/seawater hydrogen evolution. *J. Colloid Inter. Sci.* **650**, 807-815 (2023).
59. Hongjiao Huang, Aoming Huang, Di Liu, Wentao Han, Chun-Han Kuo, Han-Yi Chen, Linlin Li, **Hui Pan**, and Shengjie Peng*, Tailoring oxygen reduction reaction kinetics on perovskite oxides via oxygen vacancies for low-temperature and knittable zinc–air batteries. *Adv. Mater.* **35**, 2303109 (2023).
60. Di Liu, Lulu Qiao, Shuyang Peng, Haoyun Bai, Chunfa Liu, Weng Fai Ip, Kin Ho Lo, Hongchao Liu, Kar Wei Ng, Shuangpeng Wang*, Xiaozhan Yang, and **Hui Pan***, Recent advances in

- electrocatalysts for efficient nitrate reduction to ammonia. *Adv. Funct. Mater.* **33**, 2303480 (2023).
61. Liming Deng, Shuyi Liu, Di Liu, Yu-Ming Chang, Linlin Li, Chunsheng Li, Yan Sun, Feng Hu*, Han-Yi Chen, **Hui Pan***, and Shengjie Peng*, Activity-Stability Balance: The Role of Electron Supply Effect of Support in Acidic Oxygen Evolution, *Small* **19**, 2302238 (2023).
 62. Pengfei Zhou, Songbo Chen, Haoyun Bai, Chunfa Liu, Jinxian Feng, Di Liu, Lulu Qiao, Shuangpeng Wang*, and **Hui Pan***, Facile formation of Zn-incorporated NiFe layered double hydroxide as highly-efficient oxygen evolution catalyst. *J. Colloid Inter. Sci.* **647**, 65-72 (2023).
 63. Yutong Li, Bowen Li, Haoyun Bai, Zhichao Yu, Chi Tat Kwok* and **Hui Pan***, Magnetic and Electronic Properties of 2D MSX (M = Ti, V, Co and Ni, X = Br and I), *Phys. Chem. Chem. Phys.* **25**, 18691 - 18697 (2023).
 64. Liming Deng, Shuyi Liu, Di Liu, Yu-Ming Chang, Linlin Li, Chunsheng Li, Yan Sun, Feng Hu*, Han-Yi Chen, **Hui Pan***, and Shengjie Peng*, Activity-Stability Balance: The Role of Electron Supply Effect of Support in Acidic Oxygen Evolution. *Small*, 2302238 (2023).
 65. Chengqun Xu*, Haiyang Liu, Dongyu Wang, Dezhi Li, Ying Zhang, Xiaolu Liu, Jingyao Huang, Shengquan Wu, Donghua Fan, Hongguang Liu*, and **Hui Pan***, Molten-salt assisted synthesis of Polymeric Carbon Nitride-based photocatalyst for enhanced photocatalytic activity under green light irradiation. *Appl. Catal. B* **334**, 122835 (2023).
 66. Jinxian Feng, Junyan Li, Lulu Qiao, Dong Liu, Pengfei Zhou, Jun Ni and **Hui Pan***, Reconstructed Anti-Poisoning Surface for Enhanced Electrochemical CO₂ Reduction on Cu-Incorporated ZnO. *Appl. Catal. B* **330**, 122665 (2023).
 67. Mingpeng Chen, Di Liu, Lulu Qiao, Pengfei Zhou, Jinxian Feng, Kar Wei Ng, Qingju Liu*, Shuangpeng Wang* and **Hui Pan***, In-situ/operando Raman techniques for in-depth understanding on electrocatalysis. *Chem. Eng. J.* **461**, 141939 (2023).
 68. Di Liu, Lulu Qiao, Yuyun Chen, Pengfei Zhou, Jinxian Feng, Chon Chio Leong, Kar Wei Ng, Shengjie Peng, Shuangpeng Wang*, Weng Fai Ip, and **Hui Pan***, Electrocatalytic Reduction of Nitrate to Ammonia on Low-Cost Manganese-incorporated Co₃O₄ nanotubes. *Appl. Catal. B* **324**, 122293 (2023).
 69. Jinxian Feng, Lulu Qiao, Pengfei Zhou, Haoyun Bai, Chunfa Liu, Chon Chio Leong, Yu-Yun Chen, Weng Fai Ip, Jun Ni, and **Hui Pan***, Nanocrystalline CoO_x glass for highly-efficient alkaline hydrogen evolution reaction. *J. Mater. Chem. A* **11**, 316-329 (2023).
 70. Jiwei Li, Junli Xu, Jia Zhao, Yixin Fang, Congcong Du, Xingyu Ding, Jinyu Ye, Yifei Sun, Kelvin HL Zhang, Shunji Xie, Jianyu Huang, Mikhail Salaev, Grigory Mamontov, Weng Fai Ip, **Hui Pan**, Sen Lin*, Haifeng Xiong*, Modulation of oxygen-etching for generating nickel single atoms for efficient electroreduction of CO₂ to syngas (CO/H₂). *J. Catal.* **421**, 332-341 (2023).
 71. Jinxian Feng, Xiongwei Zhong, Mingpeng Chen, Pengfei Zhou, Lulu Qiao, Haoyun Bai, Dong Liu, Di Liu, Yu-Yun Chen, Weng Fai Ip, Shi Chen, Jun Ni, Detao Liu, and **Hui Pan***, Iron-incorporated Defective Graphite by in-situ Electrochemical Oxidization for Oxygen Evolution Reaction. *J. Power Sources* **561**, 232700 (2023).
 72. Pengfei Zhou, Haoyun Bai, Jinxian Feng, Di Liu, Lulu Qiao, Chunfa Liu, Shuang-Peng Wang*, and **Hui Pan***, Recent Progress on bulk Fe-based alloy for industrial alkaline water electrolysis. *J. Mater. Chem. A* **11**, 1551 - 1574 (2023).
 73. Haoyun Bai, Jinxian Feng, Di Liu, Pengfei Zhou, Rucheng Wu, Chi Tat Kwok, Weng Fai Ip, Wenlin Feng, Xulei Sui, Hongchao Liu*, and **Hui Pan***, Advances in Spin Catalysts for Oxygen Evolution and Reduction Reactions, *Small* **19**, 2205638 (2023). (Hot Topic: Magnetic Materials)
 74. Lulu Qiao, Anquan Zhu, Di Liu, Jinxian Feng, Yuyun Chen, Mingpeng Chen, Pengfei Zhou, Lihong Yin, Rucheng Wu, Kar Wei Ng*, and **Hui Pan***, Crystalline phosphides/amorphous oxides composite for energy-saving hydrogen production assisted by efficient urea oxidation reaction. *Chem. Eng. J* **454**, 140380 (2023).

75. Chengqun Xu*, Dezhi Li, Haiyang Liu, Dongyu Wang, Xiaolu Liu, Shiyin Lin, Yuchen Yang, Donghua Fan, and **Hui Pan***, Construction of 1D/0D CdS nanorods/Ti₃C₂ QDs Schottky heterojunctions for efficient photocatalysis. *J. Environ. Chem. Eng.* **11**, 109191 (2023).
76. Di Liu, Jia Zhao, Youchao Kong, Haoqiang Ai, Haoyun Bai, Chon Chio Leong, Kin Ho Lo, Shuangpeng Wang*, Weng Fai Ip, Sen Lin, and **Hui Pan***, Comprehensive Mechanism for CO Electroreduction on Dual-Atom-Catalyst-Anchored N-Doped Graphene. *ChemPhysChem* **24**, e202200937 (2023).
77. Bowen Li, Haoyun Bai, Shiyong Shen, Kar Wei Ng*, and **Hui Pan***, Tunable Interstitial Anionic Electrons in Layered MXenes. *J. Phys. Condens. Matter* **35**, 034001 (2023).
78. Pengfei Zhou, Po Kee Wong, Pengda Niu, Mingpeng Chen, Chi Tat Kwok, Yuxin Tang*, Ruidi Li*, Shuangpeng Wang*, and **Hui Pan***, Anodized AlCoCrFeNi high-entropy alloy for alkaline water electrolysis with ultra-high performance. *Sci. China Mater.* **66**, 1033-1041 (2023).
79. Rui Wang, Yang Yang, Xiaocheng Xu, Sijie Chen, Alex Trukhanov, Ruiying Wang, Lianyi Shao*, Xia Lu*, Hui Pan*, and Zhipeng Sun*, Interface engineering and heterometal-doped FeOOH/Ga-Ni₃S₂ nanosheet arrays for efficient electrocatalytic oxygen evolution. *Inorg. Chem Front.* **10**, 1348-1356 (2023).
80. Mingrui Shao, Di Liu, Jinxuan Lu, Xiaofei Zhao, Jing Yu, Chao Zhang, Baoyuan Man*, Hui Pan*, and Zhen Li*, Giant enhancement of the initial SERS activity for plasmonic nanostructures via pyroelectric PMN-PT. *Nanoscale Hori.* **8**, 948-957 (2023).
81. Baoqiang Du, Jibing Tan, Chang Ji, Mingrui Shao, Xiaofei Zhao, Jing Yu, Chao Zhang, Chuansong Chen, **Hui Pan***, Baoyuan Man*, and Zhen Li*, Study of thermoelectric enhanced SERS and photocatalysis with ZnO-metal nanorod arrays. *Nano Research* **16**, 5427-5435 (2023).
82. Zhiqin Ying, Xi Yang, Jingming Zheng, Jingsong Sun, Jingwei Xiu, Yudong Zhu, Xinlong Wang, Ying Chen, Xin Li, Jiang Sheng, Chunhui Shou, Yuheng Zeng, Hui Pan*, Jichun Ye*, Zhubing He*, Bathocuproine: Ag Complex Functionalized Tunneling Junction for Efficient Monolithic Perovskite/TOPCon Silicon Tandem Solar Cell. *Solar RRL* **6**, 2200793 (2002).
83. Yang Li, Jin-Feng Liao*, **Hui Pan***, and Guichuan Xing*, Interfacial Engineering for High-Performance PTAA-Based Inverted 3D Perovskite Solar Cells. *Solar RRL* **6**, 2200647 (2002).
84. Haoyun Bai, Di Liu, Pengfei Zhou, Jinxian Feng, Xulei Sui, Yunhao Lu, Hongchao Liu* and **Hui Pan***, Spin evolution and flip in the oxygen reduction reaction: a theoretical study of Cu(Ni)XP₂S₆ (X = In, Bi and Cr). *J. Mater. Chem. A* **10**, 25262-25271 (2022).
85. Chengqun Xu*, Xiaolu Liu, Haiyang Liu, Dezhi Li, Yuchen Yang, Shiyin Lin, Donghua Fan and **Hui Pan***, Molecular engineering for constructing a D–A system and enhancing delocalization in g-C₃N₄ with superior photocatalytic activity. *J. Mater. Chem. A* **10**, 21031-21043 (2022).
86. Junnan Song, Sheng Zhao, Di Liu, Yixing Xiong, Feng Hu, Linlin Li, Lei Li, **Hui Pan***, and Shengjie Peng*, Plasma-induced defect engineering of porous metal–organic framework nanosheet arrays for efficient water splitting. *Chem. Commun.* **58**, 9662-9665 (2022).
87. Luqi Wang, Hanzhi Yu, Sheng Zhao, Hui Ma, Linlin Li, Feng Hu, Lei Li, **Hui Pan**, KM El-Khatib, and Shengjie Peng*, Electronic modulation of cobalt–molybdenum oxide via Te doping embedded in a carbon matrix for superior overall water splitting. *Inorganic Chem. Frontier* (2022).
88. Rucheng Wu, Di Liu, Jiazhong Geng, Haoyun Bai, Feifei Li, Pengfei Zhou, and **Hui Pan***, Electrochemical reduction of CO₂ on single-atom catalysts anchored on N-terminated TiN (111): Low overpotential and high selectivity. *App. Sur. Sci.* **602**, 154239 (2022).
89. Mingpeng Chen, Di Liu, Jinxian Feng, Pengfei Zhou, Lulu Qiao, Wenlin Feng, Yuyun Chen, Kar Wei Ng, Shuangpeng Wang*, Weng Fai Ip, and **Hui Pan***, In-situ generation of Ni-CoOOH through deep reconstruction for durable alkaline water electrolysis. *Chem. Eng. J.* **443**, 136432 (2022).

90. Haoyun Bai, Qingyun Wu, Haoqiang Ai, Di Liu, Jinxian Feng, Lay Kee Ang, Yunhao Lu, Ming Yang* and **Hui Pan***, Interlayer-Incorporation of MoS₂ (TM-MoS₂) to achieve unique magnetic and electronic properties for spintronics. *Adv. Electro. Mater* **8**, 2200209 (2022).
91. Chao Peng*, Tao Zhou, Ping Wei, Xiqiang Yan*, Youchao Kong, Wenkang Xu, Hongjuan Wang, Hao Yu, Jianbo Jia, Kun Zhang, Bingpu Zhou, and Hui Pan*, Steering interfacial charge kinetics: Synergizing cocatalyst roles of Ti₃C₂M_x (MXene) and NCDs for superior photocatalytic performance over TiO₂. *Appl. Sur. Sci.* **599**, 154001 (2022).
92. Haoyun Bai, Shiyong Shen, Feifei Li, Jiazhong Geng, Wenlin Feng, Hongchao Liu*, Weng Fai Ip, Yunhao Lu, and **Hui Pan***, M₄B₆X₆ as a New Family of High-Efficient Electrocatalysts: The Role of Surface Reconstruction in Water Oxidization. *ChemSusChem* **15**, e202200280 (2022).
93. Xuejian Du, Di Liu, Keyu An, Shouzhen Jiang, Zhixian Wei, Shuangpeng Wang, Weng Fai Ip, and **Hui Pan***, Advances in oxide semiconductors for surface enhanced Raman scattering. *Appl. Mater. Today* **29**, 101563 (2022).
94. Jiazhong Geng, Rucheng Wu, Haoyun Bai, Iat-Neng Chan, Kar Wei Ng*, Weng Fai Ip, and **Hui Pan***, Design of functionalized double-metal MXenes (M₂M'C₂T₂: M= Cr, Mo, M'= Ti, V) for magnetic and catalytic applications. *Int. J. Hydro. Energy* **47**, 18725-18737 (2022).
95. Keyu An, Mingpeng Chen, Bingchen He, Haoqiang Ai, Wei Wang, Zhihong Zhang, Zhongbin Pan, Shi Chen, Weng Fai Ip, Kin Ho Lo, Jianwei Chai, Shijie Wang, Ming Yang*, Shuangpeng Wang*, and **Hui Pan***, Wafer-Scale 2H-MoS₂ Monolayer for High Surface-enhanced Raman Scattering Performance: Charge-Transfer Coupled with Molecule Resonance. *Adv. Mater. Tech.* **2200217** (2022).
96. Jinxian Feng, Mingpeng Chen, Pengfei Zhou, Di Liu, Yu-Yun Chen, Bingchen He, Haoyun Bai, Dong Liu, Weng Fai Ip, Shi Chen, Detao Liu, Wenlin Feng, Jun Ni, and **Hui Pan***, Reconstruction optimization of distorted FeOOH/Ni hydroxide for enhanced oxygen evolution reaction. *Mater. Today Energy* **27**, 101005 (2022).
97. Xinyu Du, Mingpeng Chen, Shiyong Shen, Pengfei Zhou, Kin Ho Lo*, and Hui Pan*, Toward Enhanced Oxygen Evolution on NaBH₄ Treated Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-δ} Nanofilm: Insights into the Facilitated Surface Reconstruction. *Mater. Today Energy* **27**, 101563 (2022).
98. Pengfei Zhou, Pengda Niu, Jishan Liu, Nian Zhang, Haoyun Bai, Mingpeng Chen, Jinxian Feng, Di Liu, Litong Wang, Shi Chen, Chi Tat Kwok, Yuxin Tang*, Ruidi Li*, Shuangpeng Wang*, and **Hui Pan***, Anodized steel: the most promising bifunctional electrocatalyst for alkaline water electrolysis in industry. *Adv. Funct. Mater.* **32**, 2202068 (2022).
99. Haoqiang Ai, Feifei Li, Haoyun Bai, Dong Liu, Kin Ho Lo*, Shengyuan A. Yang, Yoshiyuki Kawazoe, and **Hui Pan***, Ferroelectricity Co-existed with p-Orbital Ferromagnetism and Metallicity in Two-Dimensional Metal Oxynitrides. *NPJ Comput. Mater.* **8**, 60 (2022).
100. Feifei Li, Haoqiang Ai, Shiyong Shen, Jiazhong Geng, Kin Ho Lo, and **Hui Pan***, Two-Dimensional Dirac Nodal Line Carbon Nitride to Anchor Single-Atom Catalyst for Oxygen Reduction Reaction. *ChemSusChem* **15**, e202102537 (2022).
101. Mingpeng Chen, Di Liu, Yuyun Chen, Dong Liu, Xinyu Du, Jinxian Feng, Pengfei Zhou, Baoye Zi, Qingju Liu, Kin Ho Lo, Shi Chen, Shuangpeng Wang*, Weng Fai Ip, and **Hui Pan***, Insightful view on the active sites of Ni/Ni_xP for hydrogen evolution reaction. *Appl. Mater. Today* **26**, 101343 (2022).
102. Tianwei He*, Alain R. Puente Santiago, Youchao Kong, Md Ariful Ahsan, Rafael Luque*, Aijun Du*, and **Hui Pan***, Atomically Dispersed Heteronuclear Dual-Atom Catalysts: A New Rising Star in Atomic Catalysis. *Small* **18**, 2106091 (2022).
103. Pengfei Zhou, Dong Liu, Yuyun Chen, Mingpeng Chen, Yunxiao Liu, Shi Chen, Chi Tat Kwok, Yuxin Tang*, Shuangpeng Wang*, and **Hui Pan***, Corrosion engineering boosting bulk Fe₅₀Mn₃₀Co₁₀Cr₁₀ high-entropy alloy as high-efficient alkaline oxygen evolution reaction electrocatalyst. *J. Mater. Sci. Tech.* **109**, 267-275 (2022).

104. Yang Li, Bingzhe Wang, Tanghao Liu, Qingliang Zeng, Derong Cao, **Hui Pan***, and Guichuan Xing*, Interfacial Engineering of PTAA/Perovskites for Improved Crystallinity and Hole Extraction in Inverted Perovskite Solar Cells. *ACS Appl. Mater. Interfaces* **14**, 3284-3292 (2022).
105. Ge Chen, Ziyi Dai, Sen Ding, Ming Lei, Jing Lin, Shuangpeng Wang, Yinning Zhou, **Hui Pan**, Bingpu Zhou*, Realization of integrative hierarchy by in-situ solidification of ‘semi-cured’ microcilia array in candle flame for robust and flexible superhydrophobicity. *Chem. Eng. J.* **432**, 134400 (2022).
106. Shengwen Li, Junmin Xia, Chao Liang, Zhaorui Wen, Zhen Mu, Kaiyang Wang, Hao Gu, Shiliang Mei, **Hui Pan**, Jiangzhao Chen, Guichuan Xing*, and Shi Chen*, Anion induced bottom surface passivation for high performance perovskite solar cell. *Chem. Eng. J.* **442**, 135895 (2022).
107. Chengqun Xu*, Dezhi Li, Xiaolu Liu, Renzhi Ma, Nobuyuki Sakai, Yuchen Yang, Shiyin Lin, Jiale Yang, **Hui Pan***, Janjer Huang, and Takayoshi Sasaki*, Direct Z-scheme construction of g-C₃N₄ quantum dots / TiO₂ nanoflakes for efficient photocatalysis. *Chem. Eng. J.* **430**, 132861 (2022).
108. Di Liu, Mingpeng Chen, Keyu An, Dong Liu, Yuyun Chen, Pengfei Zhou, Jielei Li, Jinxian Feng, Ye Ke, Detao Liu, Pengcheng Zhao, Chi Tat Kwok, Shi Chen, Shuangpeng Wang*, Weng Fai Ip, and **Hui Pan***, In situ surface reconstruction on LaCoO_{3-δ} leads to enhanced hydrogen evolution reaction. *J. Alloys and Compounds* **891**, 161754 (2022).
109. Mingpeng Chen, Di Liu, Baoye Zi, Yuyun Chen, Dong Liu, Xinyu Du, Feifei Li, Pengfei Zhou, Ye Ke, Jielei Li, Kin Ho Lo, Chi Tat Kwok, Weng Fai Ip, Shi Chen, Shuangpeng Wang*, Qingju Liu and **Hui Pan***, Remarkable synergistic effect in cobalt-iron nitride/alloy nanosheets for robust electrochemical water splitting. *J. Energy Chem.* **65**, 405-414 (2022).
110. Yunjian Li, Haoqiang Ai, Kin Ho Lo, Youchao Kong, **Hui Pan***, Zongjin Li, Insight into adsorption mechanism of water on tricalcium silicate from first-principles calculations. *Cement and Concrete Research* **152**, 106684 (2022).
111. Yinghui Li, Yuanju Qu, Chaocheng Liu, Jiedong Cui, Ke Xu, Yang Li, Haoyu Shen, Zhouguang Lu, **Hui Pan**, Tao Xu, Detao Liu*, Processing Agricultural Cornstalks toward High-Efficient Stable Bifunctional ORR/OER Electrocatalysts. *Adv. Sustain. Sys.* **6**, 2100343 (2022).
112. Chao Peng*, Tao Zhou, Ping Wei, Haoqiang Ai, Bingpu Zhou, **Hui Pan**, Wenkang Xu, Jianbo Jia, Kun Zhang, Hongjuan Wang, Hao Yu, Regulation of the rutile/anatase TiO₂ phase junction in-situ grown on –OH terminated Ti₃C₂T_x (MXene) towards remarkably enhanced photocatalytic hydrogen evolution. *Chem. Eng. J.* **439**, 135685 (2022).
113. Rui Tong*, Miao Xu, Haiming Huang, Jun Wu, Yongchen Xiong, Mengmeng Shao, Yunyang Zhao*, Shuangpeng Wang*, and Hui Pan, Co₃Mo₃N nanosheets arrays on nickel foam as highly efficient bifunctional electrocatalysts for overall urea electrolysis. *Int. J. Hydro. Energy* **47**, 11447-11455 (2022).
114. Rui Tong*, Miao Xu, Haiming Huang, Chuankun Zhang, Yanan Ma, Xina Wang, Xiaosai Hu*, Yuanju Qu*, Shuangpeng Wang, and **Hui Pan***, Co₂N_{0.67}/MoO₂ Heterostructure as High-Efficiency Electrocatalysts for the Hydrogen Evolution Reaction. *ACS Appl. Energy Mater.* **5**, 440–448 (2021).
115. Rui Tong*, Miao Xu, Haiming Huang, Chengrui Wu, Xiao Luo, Minglei Cao, Xingxing Li, Xiaosai Hu*, Shuangpeng Wang*, and **Hui Pan**, 3D V–Ni₃S₂@CoFe-LDH core-shell electrocatalysts for efficient water oxidation. *Int. J. Hydro. Energy* **46**, 39636-39644 (2021).
116. Hua Bai, Xinyi Li, **Hui Pan**, Pimo He, Zhu-an Xu, and Yunhao Lu*, Van der Waals Antiferroelectric Magnetic Tunnel Junction: A First-Principles Study of a CrSe₂/CuInP₂S₆/CrSe₂ Junction. *Appl. Mater. Interfaces* **13**, 60200-60208 (2021).

117. Feifei Li, Haoqiang Ai, Dong Liu, Kin Ho Lo, and **Hui Pan***, Enhanced oxygen evolution reaction on 2D CoOOH via strain engineering: an insightful view from spin state transition. *J. Mater. Chem. A* **9**, 17749 - 17759 (2021). (*Cover page article*)
118. Youchao Kong, Tianwei He*, Alain R Puente Santiago, Dong Liu, Aijun Du, Shuangpeng Wang*, and **Hui Pan***, Unravelling the Reaction Mechanisms of N₂ Fixation on Molybdenum Nitride: A Full DFT study from the Pristine Surface to Heteroatom Anchoring. *ChemSusChem* **14**, 3257-3266 (2021). (*Cover page and VIP article*)
119. Tianwei He*, You-Chao Kong, Alain Rafael Puente Santiago, Md Ariful Ahsan, **Hui Pan*** and Aijun Du*, Graphynes as Emerging 2D-Platforms for Electronic and Energy applications: A Computational Perspective, *Mater. Chem. Frontiers* **5**, 6392-6412 (2021).
120. Haoyun Bai, Haoqiang Ai, Bowen Li, Dong Liu, Kin Ho Lo, Kar Wei Ng, Xingqiang Shi, Yoshiyuki Kawazoe, and **Hui Pan***, CNSi/MXene/CNSi: Unique Structure with Specific Electronic Properties for Nanodevices. *Small* **17**, 2101482 (2021).
121. Dong Liu, Pengfei Zhou, Haoyun Bai, Haoqiang Ai, Xinyu Du, Mingpeng Chen, Di Liu, Weng Fai Ip, Kin Ho Lo, Chi Tat Kwok, Shi Chen,* Shuangpeng Wang,* Guichuan Xing,* Xuesen Wang, and **Hui Pan***, Development of perovskite oxide-based electrocatalysts for oxygen evolution reaction. *Small* **17**, 2101605 (2021). (*Cover page article*)
122. Xinyu Du, Junling Guo, Mingpeng Chen, Weng-Chon Cheong, Yuyun Chen, Dong Liu, Shi Chen, Xuesen Wang, Kin Ho Lo*, Jin-Song Hu, and **Hui Pan***, Surface reconstruction on silver nanoparticles decorated trimetallic hydroxide nanosheets to generate highly active oxygen-deficient (oxy)hydroxide layer for high-efficient water oxidation. *Chem. Eng. J* **425**, 131662 (2021).
123. Tong Yang, Yong Zheng Luo, Zishen Wang, Tao Zhu, **Hui Pan**, Shijie Wang, Shu Ping Lau, Yuan Ping Feng*, and Ming Yang*, Ag₂S monolayer: an ultrasoft inorganic Lieb lattice. *Nanoscale* **13**, 14008-14015 (2021).
124. Tianqi Deng, Wen Shi, Zicong Marvin Wong, Gang Wu*, Xiaoping Yang, Jin-Cheng Zheng, **Hui Pan**, and Shuo-Wang Yang*, Designing Intrinsic Topological Insulators in Two-Dimensional Metal–Organic Frameworks, *J. Phys. Chem. Lett.* **12**, 6934-6940 (2021).
125. Chengqun Xu*, Xiaolu Liu, Dezhi Li, Zeyuan Chen, Jiale Yang, Janjer Huang, and **Hui Pan***, The coordination of π -delocalization in g-C₃N₄ for efficient photocatalytic hydrogen evolution under visible light. *ACS Appl. Mater. Inter.* **13**, 20114–20124 (2021).
126. Lin-Bo Huang, Lu Zhao, Yun Zhang, Hao Luo, Xing Zhang, Jianan Zhang, **Hui Pan**, Jin-Song Hu*, Engineering carbon-shells of M@NC bifunctional oxygen electrocatalyst towards stable aqueous rechargeable Zn-air batteries, *Chem. Eng. J.* **418**, 129409 (2021).
127. Bowen Li, Jiazhong Geng, Haoqiang Ai, Youchao Kong, Haoyun Bai, Kin Ho Lo, Kar Wei Ng*, Yoshiyuki Kawazoe, and **Hui Pan***, Design of 2D materials – MSi₂C_xN_{4-x} (M = Cr, Mo, and W; x = 1 and 2) - with tunable electronic and magnetic properties. *Nanoscale* **13**, 8038 - 8048 (2021). (*Cover Page Article*)
128. Tianwei He, Cheng Tang, Alain R. Puente Santiago, Rafael Luque, **Hui Pan***, and Aijun Du*. Tuning CO Binding Strength via Engineering Copper/Borophene Interface for Highly Efficient Conversion of CO into Ethanol. *J. Mater. Chem. A* **9**, 13192-13199 (2021).
129. Jinxian Feng, Jun Ni and **Hui Pan***, Synergistic Carbon and Hydrogen Reactions in Electrochemical Reduction of CO₂ to Liquid Fuels. *J. Mater. Chem. A* **9**, 10546 - 10561 (2021).
130. Zhiqin Ying, Xi Yang, Jingming Zheng, Yudong Zhu, Jingwei Xiu, Wei Chen, Chunhui Shou, Jiang Sheng, Yuheng Zeng, Baojie Yan, **Hui Pan***, Jichun Ye*, Zhubing He*, Charge-transfer induced multifunctional BCP: Ag complexes for semi-transparent perovskite solar cells with a record fill-factor of 80.1%. *J. Mater. Chem. A* (2021). (*Front Cover Page Article*)
131. Dong Liu, Haoqiang Ai, Mingpeng Chen, Pengfei Zhou, Bowen Li, Di Liu, Xinyu Du, Kin Ho Lo, Kar-Wei Ng, Shuang-Peng Wang*, Shi Chen*, Guichuan Xing*, Jinsong Hu, and **Hui Pan***, Multi-phase Heterostructure of CoNiP/Co_xP for Enhanced Hydrogen Evolution

- Under Alkaline and Seawater Conditions by Promoting H₂O Dissociation. *Small* **17**, 2007557 (2021).
132. Jiazhong Geng, Keyu An, Iat-Neng Chan, Haoqiang Ai, Kin Ho Lo, Kar Wei Ng*, Yoshiyuki Kawazoe and **Hui Pan***, ab initio design of a new family of 2D materials: transition metal carbon nitrogen compounds (MCNs). *J. Mater. Chem. C* **9**, 4748 - 4756 (2021). (*Front Cover Page and Hot Article*)
 133. Pengfei Zhou, Dong Liu, Zhaorui Wen, Mingpeng Chen, Qingju Liu, Ye Ke, Shengwen Li, Shi Chen, Chi Tat Kwok, Shuangpeng Wang*, Yuxin Tang*, and **Hui Pan***, Quaternary-Metal Phosphide as Electrocatalyst for Efficient Hydrogen Evolution Reaction in Alkaline Solution. *Int. J. Hydro. Energy* **46**, 18878-18886 (2021).
 134. Feifei Li, Haoqiang Ai, Changmin Shi, Kin Ho Lo, and **Hui Pan***, Single transition metal atom catalysts on Ti₂CN₂ for efficient CO₂ reduction reaction. *Int. J. Hydro. Energy* **46**, 12886-12896 (2021).
 135. Mingyang Yang, Chaoqun Shang, Feifei Li, Chen Liu*, Zhenyu Wang, Shuai Gu, Di Liu, Lujie Cao, Junjun Zhang, Zhouguang Lu*, and **Hui Pan***, Synergistic electronic and morphological modulation on ternary Co_{1-x}V_xP nanoneedle arrays for hydrogen evolution reaction with large current density. *Science China Materials* **64**, 880-891(2021).
 136. Xiongwei Zhong, Shulong Ye, Jun Tang, Yuanmin Zhu, Duojie Wu, Meng Gu, **Hui Pan***, and Baomin Xu*, Engineering Pt and Fe Dual-Metal Single Atoms Anchored on Nitrogen-Doped Carbon with High Activity and Durability towards Oxygen Reduction Reaction for Zinc-Air Battery. *Appl. Catal. B* **286**, 119891 (2021).
 137. Haoqiang Ai, Di Liu, Jiazhong Geng, Shuangpeng Wang, Kin Ho Lo*, and **Hui Pan***, Theoretical evidence of the spin-valley coupling and valley polarization in two-dimensional MoSi₂X₄ (X = N, P, and As). *Phys. Chem. Chem. Phys.* **23**, 3144 - 3151 (2021).
 138. Yuanju Qu, Chi Tat Kwok, Yangfan Shao, Xingqiang Shi, Yoshiyuki Kawazoe, and **Hui Pan***, Pentagonal transition-metal (group X) chalcogenide monolayers: intrinsic semiconductors for photocatalysis. *Int. J. Hydro. Energy* **46**, 9371-9379 (2021).
 139. Dong Liu, Mingpeng Chen, Xinyu Du, Haoqiang Ai, Kin Ho Lo, Shuangpeng Wang*, Shi Chen*, Guichuan Xing*, Xuesen Wang, and **Hui Pan***, Development of Electrocatalysts for Efficient Nitrogen Reduction Reaction under Ambient Condition. *Adv. Funct. Mater.* **31**, 2008983 (2021).
 140. Chao Peng, Xi Xie, Wenkang Xu, Tao Zhou, Ping Wei, Jianbo Jia, Kun Zhang, Yonghai Cao, Hongjuan Wang, Feng Peng, Rui Yang*, Xiqiang Yan, **Hui Pan**, and Hao Yu*, Engineering highly active Ag/Nb₂O₅@Nb₂CT_x (MXene) photocatalysts via steering charge kinetics strategy. *Chem. Eng. J.* **421**, 128766 (2021).
 141. Youchao Kong, Shanshan Yan, Jinxian Feng, Shuangpeng Wang*, and **Hui Pan***, Design of Phosphorus-Functionalized MXenes for Highly Efficient Hydrogen Evolution Reaction. *J. Mater. Chem. A* **9**, 597 - 606 (2021).
 142. Zhongbin Pan, Jie Ding, Xu Hou, Songhan Shi, Lingmin Yao, Jinjun Liu, Peng Li, Jianwen Chen, Jiwei Zhai, and **Hui Pan***, Substantially Improved Energy Storage Capability of Ferroelectric Thin Films for Application in High-temperature Capacitors. *J. Mater. Chem. A* **9**, 9281-9290 (2021).
 143. Di Hu, Zhongbin Pan*, Xiaoyan Tan, Fan Yang, Jie Ding, Xiang Zhang, Peng Li, Jinjun Liu, Jiwei Zhai*, and **Hui Pan***, Optimization the Energy Density and Efficiency of BaTiO₃-based Ceramics for Capacitor Applications. *Chemical Engineering Journal* **409**, 127375 (2021).
 144. Weijun Miao, Zhongbin Pan*, Hanxi Chen, Xueliang Pei, Long Li, Peng Li, Jinjun Liu, Jiwei Zhai*, and **Hui Pan***, Enhancement Thermal Stability of Polyetherimide-based Nanocomposites for Applications in Energy Storage. *Composites Science and Technology* **201**, 108501 (2021).

145. Zhiqin Ying, Yudong Zhu, Xiyuan Feng, Jingwei Xiu, Rui Zhang, Xuhang Ma, Yunsheng Deng, **Hui Pan***, and Zhubing He*, Sputtered Indium-Zinc Oxide for Buffer Layer Free Semitransparent Perovskite Photovoltaic Devices in Perovskite/Silicon 4T-Tandem Solar Cells. *Adv. Mater. Interfaces* **8**, 2001604 (2021). (*Inside Front Cover*)
146. Xiyuan Feng, Qing Guo, Jingwei Xiu, Zhiqin Ying, Kar Wei Ng, Limin Huang, Shuangpeng Wang*, **Hui Pan**, Zikang Tang, and Zhubing He*, Close-loop recycling of perovskite solar cells through dissolution-recrystallization of perovskite by butylamine, *Cell Rep. Phys. Sci.* **2**, 100341 (2021).
147. Chon Chio Leong, Yuanju Qu, Yoshiyuki Kawazoe, Sut Kam Ho, and **Hui Pan***, MXenes: Novel Electrocatalysts for Hydrogen Production and Nitrogen Reduction. *Catal. Today* **370**, 2–13 (2021).
148. Dong Liu, Haoqiang Ai, Jielei Li, Mingliang Fang, Mingpeng Chen, Di Liu, Xinyu Du, Pengfei Zhou, Feifei Li, Kin Ho Lo, Yuxin Tang, Shi Chen*, Lei Wang*, Guichuan Xing*, and **Hui Pan***, Surface Reconstruction and Phase Transition on Vanadium-Cobalt-Iron Trimetal Nitrides to Form Active Oxyhydroxide for Enhanced Electrocatalytic Water Oxidation. *Adv. Energy Mater.* **10**, 2002464 (2020). (*Cover page article*)
149. Rui Tong, Kar Wei Ng, Xina Wang, Shuangpeng Wang*, Xuesen Wang, and **Hui Pan***, Two-Dimensional Materials as Novel Co-Catalysts for Efficient Solar-Driven Hydrogen Production. *J. Mater. Chem. A* **8**, 23202 - 23230 (2020).
150. Youchao Kong, Di Liu, Haoqiang Ai, Kin Ho Lo, Shuangpeng Wang*, and **Hui Pan***, Theoretical Screening of Single Atoms Supported on Two-Dimensional Nb₂CN₂ for Nitrogen Fixation. *ACS Appl. Nano Mater.* **3**, 11274–11281 (2020).
151. Yang Li, Chao Liang, Gaopeng Wang, Jielei Li, Shi Chen, Shihe Yang, Guichuan Xing*, and **Hui Pan***, Two-step solvent post-treatment on PTAA for highly efficient and stable inverted perovskite solar cells, *Photonics Research* **8**, A39-A49 (2020).
152. Fengxia Liang, Zhiqin Ying, Yi Lin, Bao Tu, Zheng Zhang, Yudong Zhu, **Hui Pan**, Haifeng Li, Linbao Luo, Oleg Ageev, Zhubing He*, High-Performance Semitransparent and Bifacial Perovskite Solar Cells with MoO_x/Ag/WO_x as the Rear Transparent Electrode, *Adv. Mater. Interfaces* **7**, 2000591(2020).
153. Hui Zhang, Li-Ming Yang*, **Hui Pan**, and Eric Ganz, Atomistic Level Mechanism of CO₂ Adsorption in N-ethylethylenediamine Functionalized M₂ (dobpdc) Metal–Organic Frameworks, *Crystal Growth & Design* **20**, 6337–6345 (2020).
154. Mingpeng Chen, Dong Liu, Xinyu Du, Kin Ho Lo, Shuangpeng Wang*, Bingpu Zhou* and **Hui Pan***, 2D Materials: Excellent substrates for Surface-enhanced Raman scattering (SERS) in chemical sensing and biosensing. *TrAC Trends in Analytical Chemistry* **130**, 115983 (2020).
155. Jinxian Feng and **Hui Pan***, Electronic State Optimization for Electrochemical N₂ Reduction Reaction in Aqueous Solution. *J. Mater. Chem. A* **8**, 13896 - 13915 (2020).
156. Qing Zhu, Yuanju Qu, Detao Liu, Kai Wei Ng*, and **Hui Pan***, Two-Dimensional Layered Materials: High-Efficient Electrocatalysts for Hydrogen Evolution Reaction. *ACS Appl. Nano Mater.* **3**, 6270–6296 (2020).
157. Xiyuan Feng, Kar Wei Ng, Shuang-Peng Wang*, Wenzhou Chen, Zhenzhong Zhang, CHEN Wei, Yunyang Zhao, Bao Tu, Zikang Tang, **Hui Pan***, and Zhubing He*, Investigation on the Role of Amines in the Liquefaction and Recrystallization Process of MAPbI₃ Perovskite. *J. Mater. Chem. A* **8**, 13585-13593 (2020).
158. Jiazhong Geng, Iat-Neng Chan, Haoqiang Ai, Kin Ho Lo, Yoshiyuki Kawazoe, Kar Wei Ng* and **Hui Pan***, Magnetic and electronic properties of 2D TiX₃ (X = F, Cl, Br and I). *Phys. Chem. Chem. Phys.* **22**, 17632 - 17638 (2020).

159. W. Chen, X. Chen, Y. Wu, G. Liu, and **Hui Pan***, First-principles investigation of ScX₂ (X= Cl, Br or I) monolayers for flexible spintronics and electronics. *Phys. Chem. Chem. Phys.* **22**, 14781-14786 (2020).
160. Qianqian Zhao, Guo Feng*, Feng Jiang*, Shanfang Lan, Junhua Chen, Feifei Zhong, Zuzhi Huang*, **Hui Pan***, Jianmin Liu, Qing Hu, and Weihui Jiang*, Nonhydrolytic sol-gel in-situ synthesis of novel recoverable amorphous Fe₂TiO₅/C hollow spheres as visible-light driven photocatalysts. *Mater. Design* **194**, 108928(2020).
161. Senchuan Huang, Yuying Meng*, Yangfei Cao, Fen Yao, Zhujie He, Xuxu Wang, Hui Pan, and Mingmei Wu*, Amorphous NiWO₄ nanoparticles boosting the alkaline hydrogen evolution performance of Ni₃S₂ electrocatalysts. *Appl. Catal. B* **274**, 119120 (2020).
162. Mingpeng Chen, Bing Ji, Ziyi Dai, Xinyu Du, Bingchen He, Ge Chen, Dong Liu, Shi Chen, Kin Ho Lo, Shuangpeng Wang*, Bingpu Zhou* and **Hui Pan***, Vertically-aligned 1T/2H-MS₂ (M= Mo, W) nanosheets for surface-enhanced Raman scattering with long-term stability and large-scale uniformity. *Appl. Surf. Sci.* **527**, 146769 (2020).
163. **Hui Pan***, Carrier-potential interaction for high-T_c superconductivity. *Int. J. Mod. Phys. B* **34**, 2050163 (2020).
164. Kai-An Tsai, P. Y. Hsieh, T. H. Lai, C. W. Tsao, **Hui Pan**, Y. G. Lin, and Yung-Jung Hsu*, Nitrogen-Doped Graphene Quantum Dots for Remarkable Solar Hydrogen Production. *ACS Appl. Energy Mater.* **6**, 5322-5332 (2020).
165. Di Liu, Haoqiang Ai, Wan Tong Lou, Feifei Li, Kin Ho Lo, Shuang-Peng Wang* and **Hui Pan***, Substrate Strain Engineering: an efficient strategy to enhance the catalytic activity of SACs on waved graphene for e-NRR, *Sustainable Energy & Fuels* **4**, 3773 - 3779 (2020).
166. Haoqiang Ai, Youchao Kong, Di Liu, Feifei Li, Jiazhong Geng, Shuang-Peng Wang, Kin Ho Lo* and **Hui Pan***, 1T^{''} Transition-Metal Dichalcogenides: Strong Bulk Photovoltaic Effect for Enhanced Solar-Power Harvesting. *J. Phys. Chem. C* **124**, 11221–11228 (2020).
167. Xinyu Du, Haoqiang Ai, Mingpeng Chen, Dong Liu, Shi Chen, Xuesen Wang, Kin Ho Lo* and **Hui Pan***, PLD-fabricated perovskite oxide nanofilm as efficient electrocatalyst with highly enhanced water oxidation performance. *Appl. Catal. B* **272**, 119046 (2020).
168. Dong Liu, Rui Tong, Yuanju Qu, Qing Zhu, Xiongwei Zhong, Mingliang Fang, Kin Ho Lo, Feifei Zhang, Yinchao Ye, Yuxing Tang, Shi Chen*, Guichuan Xing* and **Hui Pan***, Highly Improved Electrocatalytic Activity of NiS_x: Effects of Cr-doping and Phase Transition. *Appl. Catal. B* **267**, 118721 (2020).
169. Youchao Kong, Haoqiang Ai, Wei Wang, Xiuhua Xie, Kin Ho Lo, Shuang-Peng Wang*, and **Hui Pan***, Waved 2D Transition-Metal Disulfides for Nanodevices and Catalysis: A First-Principle Study. *ACS Appl. Nano Mater.* **3**, 2804-2812 (2020).
170. Wenji Ai, KH Lo*, Xiang Li, CT Kwok, and Hui Pan, Cavitation Erosion Damage Mechanism of a Duplex Stainless Steel Having a Ferrite-Austenite-Sigma-Phase Triplex Microstructure. *J. Mater. Eng. Performance* **29**, 2806-2815 (2020).
171. Rui Tong, Zhi Sun, Xina Wang, Liming Yang, Jiwei Zhai, Shuangpeng Wang*, and **Hui Pan***, Mo incorporated Ni nanosheet as high-efficiency co-catalyst for enhancing the photocatalytic hydrogen production of g-C₃N₄. *Int. J. Hydro. Energy* **45**, 18912-18921 (2020).
172. Kin Long Ao, Yangfan Shao, Iat Neng Chan, Xingqiang Shi, Yoshiyuki Kawazoe, Ming Yang, Kar Wei Ng* and **Hui Pan***, Design of Novel pentagonal 2D transitional-metal sulphide monolayers for Hydrogen Evolution Reaction. *Int. J. Hydro. Energy* **45**, 16201-16209 (2020).
173. Lujie Cao, Yangfan Shao, **Hui Pan*** and Zhouguang Lu*, Designing Efficient Dual-Metal Single-Atom Electrocatalyst TMZnN₆ (TM = Mn, Fe, Co, Ni, Cu, Zn) for Oxygen Reduction Reaction. *J. Phys. Chem. C* **124**, 11301-11307 (2020).
174. Rui Tong, Yuanju Qu, Qing Zhu, Xina Wang, Yunhao Lu, Shuangpeng Wang*, and **Hui Pan***, Combined experimental and theoretical assessment on WX_y (X=C, N, S, P) for hydrogen evolution reaction, *ACS Appl. Energy Mater.* **3**, 1082-1088 (2020).

175. Xinwei Wang, Chengcheng Xiao, Chao Yang, Miaogen Chen, Shengyuan A. Yang, Jun Hu, Zhaohui Ren, **Hui Pan**, Wenguang Zhu, Zhu-An Xu, and Yunhao Lu*, Ferroelectric control of single-molecule magnetism in 2D limit. *Sci. Bulletin* **65**, 1252-1259 (2020).
176. Hairui Bai, Guanglong Ge, Xia He, Bo Shen*, Jiwei Zhai* and **Hui Pan**, Ultrahigh breakdown strength and energy density of polymer nanocomposite containing surface insulated BCZT@BN nanofibers. *Comp. Sci. Technol.* **195**, 108209 (2020).
177. Shu Hearn Yu, Wenzhou Chen, Hongyu Wang, Haiwen Dai, Zhen Quan, Cavin Ng, **Hui Pan**, and Daniel Chua*, Engineering Sulfide-phosphide Based Double Catalysts on 3D Nickel Phosphides Framework for Electrolytic Hydrogen Evolution: Activating Short-range Crystalline MoS₂ with Ni₅P₄-Ni₂P Template. *J. Electrochem. Soc.* **167**, 026511 (2020).
178. Xiongwei Zhong, Wendi Yi, Yuanju Qu, Luozheng Zhang, Haoyu Bai, Yuanmin Zhu, Jing Wan, Shi Chen, Ming Yang, Li Huang, Meng Gu, **Hui Pan***, and Baomin Xu*, Co Single-atom Anchored on Co₃O₄ and Nitrogen-Doped Active Carbon toward Bifunctional Catalyst for Zinc-Air Batteries, *Appl. Catal. B* **260**, 118188 (2020).
179. Tianqi Deng, Yong Xue, Wen Shi, Zicong Marvin Wong, Gang Wu, **Hui Pan**, Jian-Sheng Wang, and Shuo-Wang Yang*, Beyond Mahan-Sofa Best Thermoelectric Strategy: High Thermoelectric Performance from Directional π -Conjugation in Two-Dimensional Poly (tetrathienoanthracene). *J. Mater. Chem. A* **8**, 4257–4262 (2020).
180. Limei Wen, Guoliang Li, Li-Ming Yang*, **Hui Pan**, and Eric Ganz, The Structures, Electronic Properties, and Chemical Bonding of Binary Alloy Boron–Aluminum Clusters Series B₄Al_n^{0/+} (n= 1–5). *Mater. Today Commun.* **24**, 100914 (2020).
181. Q. Guo, J. Mao, J. Huang, Z. Wang, Y. Zhang, J. Hu, J. Dong, S. Sathasivam, Y. Zhao, G. Xing, **Hui Pan**, Y. Lai*, and Y. Tang*, Reducing Oxygen Evolution Reaction Overpotential in Cobalt-Based Electrocatalysts via Optimizing the “Microparticles-in-Spider Web” Electrode Configurations. *Small*, 1907029 (2020).
182. Yangfan Shao, Qian Wang, **Hui Pan***, and Xingqiang Shi*, Van der Waals contact to 2D semiconductors with a switchable electric dipole: achieving both n- and p-type Ohmic contacts to metals with a wide range of work-functions. *Adv. Electron. Mater.*, 1900981 (2019).
183. Rui Tong, Zhi Sun, Xina Wang, Shuangpeng Wang*, and **Hui Pan***, Ultra-fine WC_{1-x} nanocrystals: an efficient cocatalyst for the significant enhancement of photocatalytic hydrogen evolution on g-C₃N₄, *J. Phys. Chem. C* **123**, 26136-26144 (2019).
184. Lujie Cao, Zhenyu Wang, Jinglong Liu, Bingxue Wang, Zhiqiang Wang, Mingyang Yang, **Hui Pan***, and Zhouguang Lu*, A novel Mn/Co dual nanoparticle decorated hierarchical carbon structure derived from biopolymer hydrogel as highly efficient electro-catalyst for oxygen reduction reaction, *Chem. Commun.* **55**, 13900-13903 (2019).
185. Zhiqin Ying, Xi Yang, Rui Tong, Qing Zhu, Tian Chen, Zhubing He*, and **Hui Pan***, Enhancing the efficiency and stability of NiO_x based silicon photoanode via interfacial engineering. *ACS Appl. Energy Mater.* **2**, 6883–6890 (2019).
186. Feifei Li, Li Chen, Hongmei Liu, Dongchao Wang, Changmin Shi* and **Hui Pan***, Enhanced N₂-fixation by Engineering the Edges of Two-dimensional Transition Metal Disulfides, *J. Phys. Chem. C* **123**, 22221–22227 (2019).
187. Qing Zhu, Lingmin Yao, Rui Tong, Dong Liu, Kar Wei Ng* and **Hui Pan***, Cobalt/Titanium Nitride@N-doped Carbon Hybrid for Enhanced Electrocatalytic Hydrogen Evolution and Supercapacitance. *New J. Chem.* **43**, 14518 - 14526 (2019).
188. Shu Hearn Yu, Zhe Tang, Yangfan Shao, Haiwen Dai, Hong Yu Wang, Jiaxin Yan, **Hui Pan**, and Daniel H. C. Chua*, In-situ hybridizing MoS₂ microflowers on VS₂ microflakes in a one-pot CVD process for electrolytic hydrogen evolution reaction. *ACS Appl. Energy Mater.* **2**, 5799-5808 (2019).
189. Peng-Lai Gong, Fang Zhang, Liang Li, Bei Deng, Hai-Feng Du, **Hui Pan***, Liang-Feng Huang*, and Xing-Qiang Shi*, Highly in-plane anisotropic two-dimensional semiconductors β -

- AuSe with multiple superior properties: a first-principles investigation. *J. Phys. Condens. Matter* **31**, 395501 (2019).
190. Mengmeng Shao, Wenzhou Chen, Shengjie Ding, Kin Ho Lo, Xiongwei Zhong, Linmin Yao, Weng Fai Ip, Baomin Xu, Xuesen Wang, and **Hui Pan***, WX_y/g-C₃N₄ (X = C, N & S) composites for highly efficient photocatalytic water splitting, *ChemSusChem* **12**, 3355 – 3362 (2019).
 191. Yangfan Shao, Penglai Gong, **Hui Pan***, and Xingqiang Shi*, H-/dT-MoS₂-on-MXene Heterostructures as Promising 2D Anode Materials for Lithium-Ion Batteries: Insights from First-Principles. *Advanced Theory and Simulations* **2**, 1900045 (2019).
 192. Mingyang Yang, Xuelian Fu, Jianqiao Zhang, Zhenyu Wang, Bingxue Wang, Liqing He, Zhiliang Wu, Hua Cheng, **Hui Pan***, and Zhouguang Lu*, Hierarchical Ultrafine Ni₃V₂O₈ Nanoparticles Anchored on rGO as High-Performance Anode Materials for Lithium-Ion Batteries, *Energy Technology* **7**, 1800784 (2019).
 193. Mingyang Yang, Xuelian Fu, Zhenyu Wang, Lujie Cao, Minchan Li, Hua Cheng, Yuchao Li, **Hui Pan***, and Zhouguang Lu*, Cobalt-Vanadium Hydroxide Nanoneedles with a Free-Standing Structure as High-Performance Oxygen Evolution Reaction Electrocatalysts. *ChemElectroChem* **6**, 2050-2055 (2019).
 194. Jia-Yi Dong, Zi-Qian Ma, Ye Yang, Shuang-Peng Wang* and **Hui Pan***, Mixed Two-Dimensional Organic-Inorganic Halide Perovskites for Highly Efficient and Stable Photovoltaic Application, *Molecules* **24**, 2144 (2019).
 195. Qing Zhu, Wenzhou Chen, Hua Cheng, Zhouguang Lu, and **Hui Pan***, WS₂ Nanosheets with Highly-Enhanced Electrochemical Activity by Facile Control of Sulphur Vacancies. *ChemCatChem* **11**, 2667-2675 (2019).
 196. Yangfan Shao, Qian Wang, Liang Hu, **Hui Pan***, and Xingqiang Shi*, BC₂N monolayer as a promising anchoring material for lithium-sulfur batteries: a first-principles study. *Carbon* **149**, 530-537 (2019).
 197. Wenzhou Chen, Ming Yang, Yi-Yang Sun, Yoshiyuki Kawazoe, Xingqiang Shi*, and **Hui Pan***, Design of pentagonal NbX monolayers for electronics and electrocatalysis, *Appl. Surf. Sci.* **479**, 595-600 (2019).
 198. Jun Chai, Zhaoyang Zheng, Hui Pan, Shengbai Zhang, K. V. Lakshmi* and Yi-Yang Sun*, Significance of hydrogen bonding networks in the proton-coupled electron transfer reactions of photosystem II from a quantum-mechanics perspective. *Phys. Chem. Chem. Phys.* **21**, 8721-8728 (2019).
 199. Jingwei Xiu, Yangfan Shao, Linxun Chen, Yue Feng, Junfeng Dai, Xusheng Zhang, Yi Lin, Yudong Zhu, Zhenggang Wu, Yini Zheng, **Hui Pan***, Chang Liu, Xingqiang Shi, Xin Cheng, and Zhubing He*, Defining the composition and electronic structure of large-scale and single-crystalline like Cs₂AgBiBr₆ films fabricated by capillary-assisted dip-coating method, *Mater. Today Energy* **12**, 186-197 (2019).
 200. Mengmeng Shao, Yangfan Shao, Shengjie Ding, Rui Tong, Xiongwei Zhong, Lingmin Yao, Weng Fai Ip, Baomin Xu, Xing-Qiang Shi, Yi-Yang Sun, Xuesen Wang, and **Hui Pan***, Carbonized MoS₂: Super-Active Co-catalyst for High-Efficient Water Splitting on CdS, *ACS Sustainable Chem. Eng.* **7**, 4220–4229 (2019).
 201. Qing Zhu, Mengmeng Shao, Shu Hearn Yu, Xina Wang, Zhe Tang, Bin Chen, Hua Cheng, Zhouguang Lu, Daniel HC Chua, and **Hui Pan***, One-Pot Synthesis of Co-Doped VSe₂ Nanosheets for Enhanced Hydrogen Evolution Reaction, *ACS Appl. Energy Mater.* **2**, 644-653 (2019).
 202. Xiongwei Zhong, Yingzhi Li, Luozheng Zhang, Jun Tang, Xiangnan Li, Chang Liu, Mengmeng Shao, Zhouguang Lu*, **Hui Pan***, and Baomin Xu*, High-Performance Sodium Ion Batteries based on Nitrogen-Doped Mesoporous Carbon Spheres with Ultrathin Nanosheets, *ACS Appl. Mater. Interfaces* **11**, 2970–2977 (2019).

203. Mingyang Yang, Lujie Cao, Zhenyu Wang, Yuanju Qu, Chaoqun Shang, Hanyu Guo, Wei Xiong, Junjun Zhang, Run Shi, Jianli Zou, Chun Cheng, **Hui Pan*** and Zhouguang Lu*, Vanadium Self-Intercalation C/V_{1.11}S₂ Nanosheets With Abundant Active Sites for Enhanced Electro-Catalytic Hydrogen Evolution, *Electrochimica Acta* **300**, 208-216 (2019).
204. Rui Tong, Zhi Sun, Xina Wang, Shuangpeng Wang*, and **Hui Pan***, Network-like Ni_{1-x}Mo_x nanosheets: multi-functional electrodes for overall water splitting and supercapacitor, *ChemElectroChem* **6**, 1338-1343 (2019). *Featured as "Cover Feature" article.*
205. Rui Tong, Zhi Sun, Xiongwei Zhong, Xina Wang, Jincheng Xu, Ye Yang, Baomin Xu, Shuangpeng Wang*, and **Hui Pan***, Enhancement of visible-light photocatalytic hydrogen production by CeCO₃OH in g-C₃N₄/CeO₂ system, *ChemCatChem* **11**, 1069-1075 (2019).
206. Hearn Yu, Wenzhou Chen, Hongyu Wang, **Hui Pan**, and Daniel H. C. Chua*, Highly Stable Tungsten Disulfide Supported on a Self-Standing Nickel Phosphide Foam as a Hybrid Electrocatalyst for Efficient Electrolytic Hydrogen Evolution, *Nano Energy* **55**, 193-202 (2019).
207. Xiaonan Zhang, Huiyu Yang, Zhiguo Jiang, Yong Zhang, Shuxiang Wu, **Hui Pan**, Nasir Khisro, and Xinman Chen*, Photoresponse of Nonvolatile Resistive Memory Device Based on All-Inorganic Perovskite CsPbBr₃ Nanocrystals, *J. Phys. D: Appl. Phys.* **52**, 125103 (2019).
208. Wenzhou Chen, Xianhua Hou, Xingqiang Shi* and **Hui Pan***, Two-Dimensional Janus transition metal oxides and chalcogenides: multifunctional properties for photocatalysts, electronics and energy conversion, *ACS Appl. Mater. Interfaces* **10**, 35289–35295 (2018).
209. Rui Tong, Zhi Sun, Fang Zhang, Xina Wang, Jingchen Xu, Xingqiang Shi, Shuangpeng Wang*, and **Hui Pan***, N and V Coincorporated Ni Nanosheets for Enhanced Hydrogen Evolution Reaction, *ACS Sustainable Chem. Eng.* **12**, 16525-16531 (2018).
210. Yuanju Qu, Ye Ke, Yangfan Shao, Wenzhou Chen, Chi Tat Kwok, Xingqiang Shi and **Hui Pan***, Effect of curvature on the hydrogen evolution reaction of graphene, *J. Phys. Chem. C* **122**, 25331-25338 (2018).
211. Mengmeng Shao, Yangfan Shao, Shengjie Ding, Jingwei Wang, Jinchen Xu, Yuanju Qu, Xiongwei Zhong, Xinman Chen, Weng Fai Ip, Ning Wang, Baomin Xu, Xingqiang Shi, Xuesen Wang, and **Hui Pan***, Vanadium disulfide decorated graphitic carbon nitride for super-efficient solar-driven hydrogen evolution, *Appl. Catal. B: Environmental* **237**, 295-301 (2018).
212. P. L. Gong, Fang Zhang, Liang-Feng Huang, Hu Zhang, Liang Li, Ruichun Xiao, Bei Deng*, **Hui Pan**, and Xingqiang Shi*, Multifunctional two-dimensional semiconductors SnP₃ universal mechanism of layer-dependent electronic phase transition, *J. Phys.: Condens. Matter* **30(47)**, 475702 (2018).
213. Yangfan Shao, Mengmeng Shao, Yoshiyuki Kawazoe, Xingqiang Shi*, and **Hui Pan***, Exploring new two-dimensional monolayers: pentagonal transitional metal borides/carbides (penta-TMB/Cs), *J. Mater. Chem. A* **6**, 10226–10232 (2018). *Featured as "Back Cover" article and selected as a Hot Article on the journal for 2018.*
214. Hedong Chen, Shaofeng Wang, Xiaojing Liu, Xianhua Hou*, Fuming Chen, **Hui Pan**, Haiqing Qin, Kwok-ho Lam*, Yingchun Xia, Guofu Zhou*, Double-coated Si-based composite composed with carbon layer and graphene sheets with void spaces for lithium-ion batteries, *Electrochimica Acta* **288**, 134-143 (2018).
215. Wenzhou Chen, Yoshiyuki Kawazoe, Xingqiang Shi* and **Hui Pan***, Two-dimensional pentagonal CrX (X = S, Se or Te) monolayers: Antiferromagnetic semiconductors for spintronics and photocatalysts, *Phys. Chem. Chem. Phys.* **20**, 18348 - 18354 (2018).
216. Jingjing Zhou, Yongsheng Guo, Chengdu Liang, Lujie Cao, **Hui Pan**, Jun Yang* and Jiulin Wang*, A new ether-based electrolyte for lithium sulfur batteries using a S@pPAN cathode, *Chem. Commun.* **43**, 5478-5481 (2018).
217. Xuexue Pan, Fengzhen Ji, Qiuyu Xia, Xinman Chen*, **Hui Pan**, Said Nasir Khisro, Shixiong Luo, Ming Chen, Yong Zhang, High-performance supercapacitors based on superior

- Co₃O₄ nanorods electrode for integrated energy harvesting-storage system, *Electrochimica Acta* **282**, 905-912 (2018).
218. Mengmeng Shao, Yangfan Shao, Wenzhou Chen, Kin Long Ao, Rui Tong, Qing Zhu, Iat Neng Chan, Weng Fai Ip, Xingqiang Shi and **Hui Pan***, Efficient nitrogen fixation to ammonia on MXenes, *Phys. Chem. Chem. Phys.* **20**, 14504 - 14512 (2018).
219. Wenzhou Chen, Yuanju Qu, Lingmin Yao, Xianhua Hou, Xingqiang Shi* and **Hui Pan***, Magnetic, Catalytic, and Electrochemical properties of Two-Dimensional Janus Transition Metal Chalcogenides, *J. Mater. Chem. A* **6**, 8021 - 8029 (2018).
220. Xiongwei Zhong, Jun Tang, Jingwei Wang, Mengmeng Shao, Jianwei Chai, Shuangpeng Wang, Ming Yang, Ye Yang, Ning Wang, Shijie Wang, Baomin Xu * and **Hui Pan***, 3D heterostructured pure and N-Doped Ni₃S₂/VS₂ nanosheets for high efficient overall water splitting, *Electrochimica Acta* **269**, 55-61 (2018).
221. Zi-Qian Ma, Yangfan Shao, Pak Kin Wong, Xingqiang Shi, and **Hui Pan***, Structural and Electronic Properties of Two-Dimensional Organic-inorganic Halide Perovskites and their Stability against Moisture. *J. Phys. Chem. C* **112**, 5844-5853 (2018).
222. Yangfan Shao, Rui Pang, **Hui Pan***, and Xingqiang Shi*, Fullerene/layered antiferromagnetic reconstructed spinterface: subsurface layer dominates molecular orbitals' spin-split and large induced magnetic moment. *J. Chem. Phys.* **148**, 114704 (2018).
223. Zishuai Zhang, Xiaoqiao Hu, Zhou Yu, Shaofeng Wang, Lingmin Yao, **Hui Pan**, Ching Yuan Su, Fuming Chen, and Xianhua Hou*, Aqueous rechargeable dual-ion battery based on fluoride ion and sodium ion electrochemistry, *J. Mater. Chem. A* **6**, 8244–8250 (2018).
224. Yangfan Shao, Xingqiang Shi*, and **Hui Pan***, Electronic, Magnetic, and Catalytic Properties of Thermodynamically Stable Two-Dimensional Transition-Metal Phosphides. *Chem. Mater.* **29**, 8892–8900 (2017).
225. Yangfan Shao, Fang Zhang, Xingqiang Shi*, and **Hui Pan***, N-functionalized MXenes: Ultrahigh carrier mobility and multifunctional properties. *Phys. Chem. Chem. Phys.* **19**, 28710 – 28717(2017).
226. Xiongwei Zhong, Linfei Zhang, Jun Tang, Jianwei Chai, Jincheng Xu, Lujie Cao, Mingyang Yang, Ming Yang, Weiguang Kong, Shijie Wang, Hua Cheng, Zhouguang Lu, Chun Cheng, Baomin Xu* and **Hui Pan***, Efficient coupling of a hierarchical V₂O₅@Ni₃S₂ hybrid nanoarray for pseudocapacitors and hydrogen production. *J. Mater. Chem. A* **5**, 17954 – 17962 (2017).
227. Mengmeng Shao, Yangfan Shao, Jianwei Chai, Yuanju Qu, Mingyang Yang, Zeli Wang, Ming Yang, Weng Fai Ip, Chi Tat Kwok, Xingqiang Shi, Zhouguang Lu, Shijie Wang, Xuesen Wang, and **Hui Pan***, Synergistic Effect of 2D Ti₂C and g-C₃N₄ for efficient photocatalytic hydrogen production. *J. Mater. Chem. A*, **5**, 16748–16756 (2017).
228. Yuanju Qu, Mengmeng Shao, Yangfan Shao, Mingyang Yang, Jincheng Xu, Chi Tat Kwok, Xingqiang Shi, Zhouguang Lu, and **Hui Pan***, Ultra-high electrocatalytic activity of VS₂ nanoflowers for efficient hydrogen evolution reaction. *J. Mater. Chem. A*, **5**, 15080 - 15086 (2017).
229. Wenzhou Chen, Haifeng Li*, Xingqiang Shi, and **Hui Pan***, Tension-tailored electronic and magnetic switching of 2D Ti₂NO₂. *J. Phys. Chem. C* **121**, 25729–25735 (2017).
230. Lujie Cao, Mingyang Yang, Zhouguang Lu* and **Hui Pan***, Exploring an effective oxygen reduction reaction catalyst via 4e- process based on waved-graphene. *Science China Materials*, **60**(8), 739–746 (2017).
231. **Hui Pan***, Waved graphene: Unique structure for the adsorption of small molecules. *Mater. Chem. Phys.* **189**, 111–117 (2017).
232. Yuanju Qu, Mingyang Yang, Jianwei Chai, Zhe Tang, Chi Tat Kwok, Ming Yang, Zhenyu Wang, Daniel Chua, Shijie Wang, Zhouguang Lu and **Hui Pan***, Facile Synthesis of

- Vanadium-Doped Ni₃S₂ Nanowire Arrays as Active Electrocatalyst for Hydrogen Evolution Reaction. *ACS Appl. Mater. Interfaces* **9**, 5959–5967 (2017).
233. Xiongwei Zhong, Jun Tang, Lujie Cao, Weiguang Kong, Zheng Sun, Hua Cheng, Zhouguang Lu, **Hui Pan***, and Baomin Xu*, Cross-linking of polymer and ionic liquid as high-performance gel electrolyte for flexible solid-state supercapacitor. *Electrochimica Acta* **244**, 112–118 (2017).
234. Xianyuan Wu, Zheng Fang, **Hui Pan**, Yifan Zheng, Dahao Jiang, Jun Ni* and Xiaonian Li*, Active oxygen species on Mg–La mixed oxides: the effect of Mg and La oxide interactions. *Catal. Sci. Technol.* **7**, 797-801 (2017).
235. Zisheng Wang* and **Hui Pan**, Exploration of CPT violation via time-dependent geometric quantities embedded in neutrino oscillation through fluctuating matter. *Nuclear Phys. B* **915**, 414-430 (2107).
236. Lujie Cao, Mingyang Yang, Dong Wu, Fucong Lyu, Zhifang Sun, Xiongwei Zhong, **Hui Pan**, Hongtao Liu and Zhouguang Lu*, Biopolymer-Chitosan based supramolecular hydrogels as solid state electrolyte for electrochemical energy storage. *Chem. Communication* **53**, 1615-1618 (2017).
237. **Hui Pan***, Ultra high electrochemical catalytic activity of MXenes. *Scientific Reports* **6**, 32531 (2016).
238. Yuanju Qu, **Hui Pan***, and Chi Tat Kwok, Hydrogenation-controlled phase transition on two-dimensional transition metal dichalcogenides and their unique physical and catalytic properties. *Scientific Reports* **6**, 34186 (2016).
239. **Hui Pan***, Principles on design and fabrication of nanomaterials as photocatalyst for water-splitting. *Renew. Sustain. Energy Rev.* **57**, 584–601 (2016).
240. **Hui Pan***, Tension-Enhanced Hydrogen Evolution Reaction on Vanadium Disulfide Monolayer. *Nanoscale Res. Lett.* **11**, 113 (2016).
241. Zi-Qian Ma, **Hui Pan***, and Pak Kin Wong, A first-principles study on the structural and electronic properties of Sn-based organic-inorganic halide perovskites. *J. Electro. Mater.* **45(11)**, 5956-5966 (2016).
242. Chon Chio Leong, **Hui Pan***, and Sut Kam Ho, Two-Dimensional Transition-Metal Oxides Monolayers as Cathode Materials for Li and Na Ion Batteries. *Phys. Chem. Chem. Phys.* **18**, 7527-7534 (2016).
243. Chao-Yao Yang, Kuan-Chang Chiu, Shu-Jui Chang, Xin-Quan Zhang; Jaw-Yeu Liang, Chi-Sheng Chung, **Hui Pan**, Jenn-Ming Wu, Yuan-Chieh Tseng*, and Yi-Hsien Lee, Phase-driven Magneto-electrical Characteristics of Single-layer MoS₂, *Nanoscale* **8**, 5627-5633 (2016).
244. Bing Xie, G. R. Zeng, **Hui Pan***, and Zisheng Wang*, Pancharatnam Phase and Quantum Correlation for Two-qubit System in Correlated Dephasing Environment. *Int. J. Theo. Phys.* **55**, 1474-1491 (2016).
245. Liyuan Xue, Yanxia Yu, **Hui Pan*** and Zisheng Wang*, Geometric phases and quantum correlations of superconducting two-qubit system with dissipative effect. *Physica C* **520**, 8-18 (2016).
246. Guolan Fu, **Hui Pan***, and Zisheng Wang*, Transition of Berry Phase and Pancharatnam Phase and Phase Change, *Int. J. Theo. Phys.* **55**, 3428–3439 (2016).
247. Yuanju Qu and **Hui Pan***, Perspective of Transition Metal Dichalcogenide Monolayers as Catalysts in Water Electrolysis. *Journal of Applied and Theoretical Physics Research* **1**, 14-15 (2016). (Editorial)
248. Enyi Ye, Michelle D. Regulacio Madurai S. Bharathi, **Hui Pan**, Ming Lin, Michel Bosman, Khin Yin Win, Hariharaputran Ramanarayan, Shuang-Yuan Zhang, Xian Jun Loh, Yong-Wei Zhang and Ming-Yong Han, An experimental and theoretical investigation of the anisotropic branching in gold nanocrosses. *Nanoscale* **8**, 543-552 (2016).

249. **Hui Pan***, Electronic Properties and Lithium Storage Capacities of Two-Dimensional Transition-Metal Nitrides Monolayers. *J. Mater. Chem. A* **3**, 21486-21493 (2015). *Selected as a Hot Article on the journal for 2015.*
250. Yuanju Qu, **Hui Pan***, Chi Tat Kwok, and Zisheng Wang, Effect of Doping on Hydrogen Evolution Reaction of Vanadium Disulfide Monolayer. *Nanoscale Res. Lett.* **10**, 480 (2015).
251. Yuanju Qu, **Hui Pan***, Chi Tat Kwok, and Zisheng Wang, A First-Principles Study on Hydrogen Evolution Reaction of VS₂ Nanoribbons. *Phys. Chem. Chem. Phys.* **17**, 24820–24825 (2015).
252. Jun Fang, Bin Chen*, and **Hui Pan***, Anomalous friction of graphene nanoribbons on waved graphenes. *Theor. Appl. Mech. Lett.* **5**, 212–215 (2015).
253. **Hui Pan*** and Xuesen Wang, Realization of Dirac Cones in Few-Bilayers Sb(111) Films by Surface Modification. *Nanoscale Res. Lett.* **10**, 334 (2015).
254. **Hui Pan***, Bandgap engineering of oxygen-rich TiO_{2+x} for photocatalyst with enhanced visible-light photocatalytic ability. *J. Mater. Sci.* **50**, 4324-4329 (2015).
255. Zisheng Wang*, Xiaoya Cai, and **Hui Pan***, Quantum simulation of trapped two-ion for neutrino electromagnetic properties in neutrino oscillation. *Nuclear Physics B* **900**, 560-575 (2015).
256. Shijie Wen, **Hui Pan***, and Yuebing Zheng, Electronic Properties of Tin Dichalcogenide Monolayers and Effects of Hydrogenation and Tension. *J. Mater. Chem. C* **3**, 3714 – 3721 (2015).
257. Zi-Qian Ma, **Hui Pan***, Zisheng Wang, and Pak Kin Wong, Effects of Non-Metal Dopants and Defects on Electronic Properties of Barium Titanate as Photocatalyst. *Int. J. Hydrogen Energy* **40**, 4766-4776(2015).
258. Qian Liu, Yanxia Yu, **Hui Pan***, and Zi-Sheng Wang*, Motion center in quantum wave packet dynamics. *Acta Physica Polonica A* **127**, 761-766 (2015).
259. Zisheng Wang* and **Hui Pan***, Geometric phase carried by the observables and its application to quantum computation. *Quantum Information and Computation* **15**, 951-961 (2015).
260. Xiaoya Cai, **Hui Pan***, and Zisheng Wang*, Geometric phase of two-qubit system in dephasing environment. *Int. J. Modern Phys. B* **29**, 1550236 (2015).
261. Yanxia Yu, **Hui Pan**, Liyuan Xue, Liping Guo*, and Zisheng Wang, Geometric phase in inhomogeneous optical nutation. *Eur. J. Phys. D* **69**, 246 (2015).
262. **Hui Pan***, Magnetic and electronic evolutions of hydrogenated VTe₂ monolayer under tension. *Scientific Reports* **4**, 7524 (2014).
263. **Hui Pan***, Metal dichalcogenides monolayers: Novel catalysts for electrochemical hydrogen production, *Scientific Reports* **4**, 5348 (2014).
264. **Hui Pan*** and Bin Chen, Ultra-flexibility and unusual electronic, magnetic, and chemical properties of waved graphenes and nanoribbons, *Scientific Reports.* **4**, 4198 (2014).
265. **Hui Pan***, Graphitic carbon nitride nanotubes as Li-ion battery materials: a first-principles study, *J. Phys. Chem. C* **118**, 9318-9323 (2014).
266. **Hui Pan***, Electronic and magnetic properties of vanadium dichalcogenides monolayers tuned by hydrogenation, *J. Phys. Chem. C* **118**, 13248–13253 (2014).
267. **Hui Pan**, *ab initio* design of nanostructures for solar energy conversion: a case study on silicon nitride nanowire. *Nanoscale Res. Lett.* **9**, 531 (2014).
268. Anna Shin Hwa Lee, Kai Li, Yong-Wei Zhang, and **Hui Pan***, *ab initio* study on the effects of dopant-defect cluster on the electronic properties of TiO₂-based photocatalysts, *Int. J. Hydro. Energy* **39**, 2049-2055 (2014).
269. Q. Liu, R-S. Wu, H. L. Xu, Y. X. Yu, **Hui Pan***, and Z-S. Wang*, Geometric phase and non-stationary state. *Optik* **125**, 4814–4818 (2014).

270. Yongqing Cai, Zhaoqiang Bai, **Hui Pan**, Yuan Ping Feng, Boris I. Yakobson* and Yong-Wei Zhang*, Constructing metallic nanoroads on a MoS₂ monolayer via hydrogenation, *Nanoscale* **6**, 1691-1697 (2014).
271. Z. D. Sha, L. C. He, Q. X. Pei, **Hui Pan**, Z. S. Liu*, Y. W. Zhang*, and T. J. Wang*, On the notch sensitivity of CuZr nanoglass. *J. Appl. Phys.* **115**, 163507 (2014).
272. Junguang Tao*, **Hui Pan**, Lai Mun Wong, Ten It Wong, J W Chai, Jisheng Pan and S J Wang*, Mechanism of insulator-to-metal transition in heavily Nb doped anatase TiO₂. *Mater. Res. Exp.* **1**, 015911 (2014).
273. Viacheslav Sorkin, **Hui Pan**, Hongliang Shi, Jerry Siu Sin Quek, Yong-Wei Zhang*, Nanoscale Transition Metal Dichalcogenides: Structures, Properties And Applications. *Critical Rev. Solid State Mater. Sci.* **39**, 319–367 (2014).
274. Kai Li, Anna Shin Hwa Lee, Yong-Wei Zhang, and **Hui Pan***, Electronic and Magnetic Properties of Silicene and Silicene Nanoribbons, *Int. J. Comput. Mater. Sci. Eng.* **2**, 1350011 (2013).
275. Hongliang Shi, **Hui Pan***, Yong-Wei Zhang*, and Boris I Yakobson, Strong ferromagnetism in hydrogenated monolayer MoS₂ tuned by strain. *Phys. Rev. B* **88**, 205305 (2013).
276. Yao Kun Lim, Eugene Wai Keong Koh, Yong-Wei Zhang, and **Hui Pan***, ab initio design of GaN-based photocatalyst: ZnO-codoped GaN nanotubes, *J. Power Sources* **232**, 323-331 (2013).
277. Hongliang Shi, **Hui Pan**, Yong-Wei Zhang*, Boris I Yakobson*, Quasiparticle band structures and optical properties of strained monolayer MoS₂ and WS₂, *Phys. Rev. B* **87**(15), 155304(2013).
278. Yanxia Yu, Guolan Fu, L.P. Guo, **Hui Pan**, Z.S. Wang*, Quantum correlations of coupled superconducting two-qubit system in various cavity environment, *Physica C* **495**, 88-108 (2013).
279. Yuanmin Du*, Amit Kumar, **Hui Pan**, Kaiyang Zeng, Shijie Wang*, Ping Yang, and Andrew Thye Shen Wee*, The resistive switching in TiO₂ films studied by conductive atomic force microscopy and Kelvin probe force microscopy, *AIP Advances* **3**, 082107 (2013). *The news on “Promising new alloy for resistive switching memory” can be found in several popular websites, such as AAAS News, Science Daily, Phys Org News, Newswise and Scicasts.*
280. **Hui Pan***, Yong-Wei Zhang, GaN-ZnO superlattice nanowires as photocatalyst for hydrogen generation-A first-principles study on electronic and magnetic properties, *Nano Energy* **1**, 488-493 (2012).
281. **Hui Pan***, Yong-Wei Zhang, Edge-dependent structure, electronic, and magnetic properties of MoS₂ nanoribbons, *J. Mater. Chem.* **22**, 7280-7290 (2012).
282. **Hui Pan***, Yong-Wei Zhang, Tuning the electronic and magnetic properties of MoS₂ nanoribbons by strain engineering, *J. Phys. Chem. C* **116**, 11752-11757 (2012).
283. Guangyong Koh, Yong-Wei Zhang, **Hui Pan***, First-principles study on hydrogen storage by graphitic carbon nitride nanotubes, *Int. J. Hydro. Energy* **37**, 4170-41789(2012). (featured on *Renewable Energy Global Innovations 2012*)
284. Eugene Wai Keong Koh, Cheng Hsin Chiu, Yao Kun Lim, Yong-Wei Zhang, and **Hui Pan***, Hydrogen adsorption on and diffusion through MoS₂ monolayer: first-principles study, *Int. J. Hydro. Energy* **37**, 14323 -14328 (2012).
285. Hualan Xu, Dan Fu, Zisheng Wang*, and **Hui Pan***, Dynamic evolution for liquid-state nuclear spins and Berry phase of mixed state in magnetic resonance, *J. Magnetic Resonance* **223**, 25-30 (2012).

286. Z.S. Wang*, Yuan-hua Li, Hualan Xu · Li-yun Hu, Yi-you Nie, L.P. Guo, Min Huang, **Hui Pan**, Observable Berry phase for charge qubit in a dissipative environment, *Int. J. Theor. Phys.* **51**, 2850–2856 (2012).
287. Yuanmin Du*, **Hui Pan**, Shijie Wang*, Tom Wu, Yuan Ping Feng, Jisheng Pan, Andrew Thye Shen Wee*, Symmetrical negative differential resistance behavior of a resistive switching device, *ACS Nano* **6**, 2517–2523 (2012).
288. Hongliang Shi, **Hui Pan**, Yong-Wei Zhang*, Boris I Yakobson*, Electronic and Magnetic Properties of Graphene/Fluorographene Superlattices, *J. Phys. Chem. C* **116**, 18278-18283 (2012).
289. Zhendong Sha*, **Hui Pan**, Q.X. Pei, Yong-Wei Zhang, The nature of the atomic-level structure in the Cu–Zr binary metallic glasses, *Intermetallics* **26**, 8-10 (2012).
290. **Hui Pan***, Yong-Wei Zhang, Vivek Shenoy, Huajian Gao, Ab Initio Study on a Novel Photocatalyst: Functionalized Graphitic Carbon Nitride Nanotube, *ACS Catalyst* **1**, 99-104 (2011).
291. **Hui Pan***, Yong-Wei Zhang, Vivek Shenoy, Huajian Gao, Effects of H, N, and (H, N) doping on the photocatalytic ability of TiO₂, *J. Phys. Chem. C* **115**, 12224-12231 (2011).
292. **Hui Pan***, Yong-Wei Zhang, Vivek Shenoy, Huajian Gao, Metal-functionalized single-walled graphitic carbon nitride nanotubes: a first-principles study on magnetic property, *Nanoscale Res. Lett.* **6**, 97 (2011).
293. **Hui Pan***, Yong-Wei Zhang, Vivek Shenoy, Huajian Gao, Ab Initio Study on the Size and Chirality Effects on the Encapsulation of Tetrafluorotetracyano-p-quinodimethane inside Carbon Nanotubes, *J. Phys. Chem. C* **115**, 5280-5285 (2011).
294. **Hui Pan***, Yong-Wei Zhang, Vivek Shenoy, Huajian Gao, Controllable magnetic property of SiC by anion-cation codoping, *Appl. Phys. Lett.* **96**, 192510 (2010).
295. **Hui Pan***, Baohua Gu, Gyula Eres, Zhenyu Zhang, Ab initio study on non-compensated CrO codoping of GaN for enhanced solar energy conversion, *J. Chem. Phys.* **132**, 104501 (2010).
296. **Hui Pan**, Yuan Ping Feng*, Jianyi Lin, Enhancement of Hydrogen Evolution on Tungsten Doped Platinum, *J. Comput. Theore. Nanosci.* **7**, 547-551 (2010).
297. **Hui Pan***, Jianyi Lin, Yuan Ping Feng, Carbon Nanotubes for Supercapacitor, *Nanoscale Res. Lett.* **5**, 654-668 (2010) (review).
298. **Hui Pan***, Baohua Gu, Zhenyu Zhang, Phase-dependent photocatalytic performance of TiO₂: a first-principles study, *J. Chem. Theory Comput.* **5**, 3074-3078 (2009).
299. **Hui Pan**, Xiaofeng Qiu, Iliia N. Ivanov, Harry M. Meyer, Wei Wang, Wenguang Zhu, M. Parans Paranthaman, Zhenyu Zhang, Gyula Eres, Baohua Gu*, Fabrication and characterization of brookite-rich, visible light-active TiO₂ films for water splitting, *Appl. Catal. B: Environ.* **93**, 90-95 (2009).
300. Wenguang Zhu, Xiaofeng Qiu, Violeta Iancu, Xing-Qiu Chen, **Hui Pan**, W. Wang, Nada M. Dimitrijevic, Tijana Rajh, Harry M. Meyer III, M. Parans Paranthaman, G. M. Stocks, Hanno H. Weitering, Baohua Gu, Gyula Eres, Zhenyu Zhang*, Band Gap Narrowing of Titanium Oxide Semiconductors by Noncompensated Anion-Cation Codoping for Enhanced Visible-Light Photoactivity, *Phys. Rev. Lett.* **103**, 226401 (2009).
301. **Hui Pan***, Yuan Ping Feng, Jianyi Lin, Symmetry Properties of Single-Walled BC₂N Nanotubes, *Nanoscale Res. Lett.* **4**, 498-502 (2009).
302. J. B. Yi*, L. Shen, **Hui Pan**, L. H. Van, S. Thongmee, J. F. Hu, Y. W. Ma, J. Ding*, Y. P. Feng, Enhancement of room temperature ferromagnetism in C-doped ZnO film by nitrogen codoping, *J. Appl. Phys.* **105**, 07C513 (2009).
303. **Hui Pan***, Chee Kok Poh, Yanwu Zhu, Guichuan Xing, Chin Kok Chung, Yuan Ping Feng, Jianyi Lin*, Chornng Haur Sow, Wei Ji, Andrew T. S. Wee, Novel CdS Nanostructures: Synthesis and Field Emission, *J. Phys. Chem. C* **112**, 11227-11230 (2008).

304. **Hui Pan**, Yuan Ping Feng*, Qin Yun Wu, Zhi Gao Huang, Jianyi Lin, Magnetic Property of Carbon Doped CdS: A First-Principles and Monte Carlo Study, *Phys. Rev. B* **77**, 125211 (2008).
305. **Hui Pan***, Yuan Ping Feng*, Jianyi Lin, *Electronic structure of Single-Wall AlGaIn₂ Nanotubes and AlN-GaN Nanotube Superlattice*, *J. Chem. Theory Comput.* **4**, 703-707 (2008).
306. **Hui Pan**, Yuan Ping Feng*, Semiconductor Nanowires and Nanotubes: Effects of Size and Surface-to-Volume Ratio, *ACS Nano* **2**, 2410-2414 (2008).
307. Lei Shen, R. Q. Wu, **Hui Pan**, G. W. Peng, M. Yang, Z. D. Sha, Yuan Ping Feng*, Mechanism of Ferromagnetism in Nitrogen-Doped ZnO: First-principles Calculations, *Phys. Rev. B* **78**, 073306 (2008).
308. **Hui Pan**, Yuan Ping Feng*, Jianyi Lin, Magnetic Properties of OH-Functionalized Carbon Nanotubes, *J. Comput. Theory Nanosci.* **5**, 2233-2237 (2008).
309. **Hui Pan***, Zhenhua Ni, Cheekok Poh, Yuan Ping Feng, Jianyi Lin, Zexiang Shen, A Simple Route to Growth of Silicon Nanowires, *J. Nanosci. Nanotechnol.* **8**, 5787-5790 (2008).
310. **Hui Pan***, Yuan Ping Feng*, Jianyi Lin, Boron Nitride and Carbon Double-Wall Hetero-Nanotubes: First-Principle Calculation of Electronic Properties, *Nanotechnology* **19**, 095707 (2008).
311. Chee Kok Poh, San Hua Lim, **Hui Pan**, Jianyi Lin*, Jim Yang Lee, Citric Acid Functionalized Multiwalled Carbon Nanotubes for Fuel Cell Applications, *J. Power Source* **176**, 70-75 (2008).
312. Jiabao Yi*, **Hui Pan***, Jianyi Lin, Jun Ding*, Yuan Ping Feng*, S. Thongmee, T. Liu, Hao Gong, Lan Wang, Ferromagnetism in ZnO Nanowires Derived from Electrodeposition on AAO Template and Subsequent Oxidation, *Adv. Mater.* **20**, 1170-1174 (2008).
313. S. Thongmee, J. Ding*, J. B. Yi, **Hui Pan**, J. B. Yi, J. Y. Lin, Aging time effect on the formation of alumina nanowires on AAO templates, *Synthesis and Reactivity in Inorganic Metal-Organic and Nano-Metal Chemistry* **38**, 469-474 (2008).
314. San Hua Lim, Jianyi Lin*, Lei Liu, **Hui Pan**, Hua Long Pan, Wei Ji, Yuan Peng Feng, Zexiang Shen, Functionalization Effect On The Electronic Properties Of Single Walled Carbon Nanotubes, *Functional Materials Letter* **1**, 1-6 (2008).
315. **Hui Pan***, Cheekok Poh, Yuan Ping Feng, Jianyi Lin*, Supercapacitor Electrodes from Tubes-in-Tube Carbon Nanostructures, *Chem. Mater.* **19**, 6120 (2007).
316. **Hui Pan***, Guichuan Xing, Zhenhua Ni, Wei Ji*, Yuan Ping Feng*, Zhe Tang, Daniel H. C. Chua, Jianyi Lin, Zexiang Shen, Stimulated Emission of CdS Nanowires Grown by Thermal Evaporation, *Appl. Phys. Lett.* **91**, 193105 (2007). Also highlighted on Virtual Journal of Nanoscale science & Technology 16 (21) (Nov. 19, 2007).
317. **Hui Pan**, Jiabao Yi, Lei Shen, Rongqin Wu, Junhua Yang, Jianyi Lin, Yuan Ping Feng*, Jun Ding*, L. H. Van, J. H. Yin, Room Temperature Dilute Magnetic Semiconductor in Carbon-Doped ZnO, *Phys. Rev. Lett.* **99**, 127201 (2007) (*highlighted by physicsworld.com* (3 Oct. 2007)).
318. **Hui Pan**, Yuan Ping Feng, Jianyi Lin*, Chuanjun Liu, Thye Shen Wee, Catalyst-Free Template-Synthesis of ZnO Nanopetals at 60 °C, *J. Nanosci. Nanotechnol.* **7**, 696-699 (2007).
319. **Hui Pan***, Yuan Ping Feng*, Jianyi Lin, Hydrogen Adsorption by Tungsten Carbide Nanotube, *Appl. Phys. Lett.* **90**, 223104(2007). Also highlighted on Virtual Journal of Nanoscale science & Technology 15 (23) (Jun. 11, 2007).
320. **Hui Pan**, Zhenhua Ni, Jiabao Yi, Xinyu Gao, Chuanjun Liu, Yuan Ping Feng*, Jun Ding, Jianyi Lin, Andrew Thye Shen Wee, Zexiang Shen, Optical and Magnetic Properties of Ni-Doped ZnO Nanocones, *J. Nanosci. Nanotechnol.* **7**, 3620-3623 (2007).
321. Hailong Zhou, **Hui Pan**, Taw Kuei Chan, Chee Sheng Ho, Yuanping Feng, Soo-Jin Chua*, Thomas Osipowicz, Channeling Contrast Microscopy of Epitaxial Lateral Overgrowth of ZnO/GaN Films, *Nuclear Instruments & Methods in Phys. Research B* **260**, 299-303 (2007).

322. Hailong Zhou, Soo-Jin Chua*, **Hui Pan**, Yanwu Zhu, Thomas Osipowicz, Wei Liu, Keyan Zang, Yuan Ping Feng, Chorng-Haur Sow, Morphology Controllable ZnO Growth on Facet-Controlled Epitaxial Lateral Overgrown GaN/Sapphire Templates, *J. Phys. Chem. C* **111**, 6405-6410 (2007).
323. Hailong Zhou, Soo-Jin Chua*, **Hui Pan**, Jianyi Lin, Yuan Ping Feng, Lianshan Wang, Wei Liu, Keyan Zang, Sudhiranjan Tripathy, Structural Properties of ZnO Grown on GaN/Sapphire Templates: Transition from Nanorods to Thin Films, *Electroch. Solid-State Lett.* **10** (3) H98-H100 (2007).
324. Hailong Zhou, Soo-Jin Chua*, S. Y. Chow, **Hui Pan**, Y.W. Zhu, Yuan Ping Feng, L. S. Wang, K. Y. Zang, W. Liu, S. Tripathy, Characteristics of Threading Dislocations in ZnO Grown on Facet-Controlled Epitaxial Overgrown GaN Templates, *J. Phys.: Condens. Matter* **19**, 356203 (2007).
325. **Hui Pan**, Yuan Ping Feng*, Jianyi Lin, *Ab Initio* Study of Single-Wall BC₂N Nanotubes, *Phys. Rev. B* **74**, 045409 (2006). Also highlighted on Virtual Journal of Nanoscale science & Technology 14 (4) (Jul. 24, 2006).
326. **Hui Pan**, Yuan Ping Feng*, Jianyi Lin, First-Principles Study of Optical Spectra of Single-Wall BC₂N Nanotubes, *Phys. Rev. B* **73**, 0345420 (2006). Also highlighted on Virtual Journal of Nanoscale science & Technology 13 (3) (Jan. 23, 2006).
327. **Hui Pan**, Weizhe Chen, Yuan Ping Feng, Wei Ji*, Jianyi Lin*, Optical Limiting of Metal Nanowires, *Appl. Phys. Lett.* **88**, 223106 (2006). Also highlighted on Virtual Journal of Nanoscale science & Technology 13 (23) (Jun 12, 2006) and *Photonics Spectra* (Aug. 1, 2006).
328. **Hui Pan**, Zhenhua Ni, Han Sun, Zhihua Yong, Yuan Ping Feng, Zexiang Shen, Andrew Thye Shen Wee, Jianyi Lin*, Strong Green Emission of Mg Doped ZnO Nanowires, *J. Nanosci. Nanotechnol.* **6**, 2529-2532 (2006).
329. **Hui Pan***, Yanwu Zhu, Han Sun, Yuan Ping Feng, Chow Haur Sow, Jianyi Lin, Electroluminescence and Field Emission Properties of Mg Doped ZnO Tetrapods, *Nanotechnology* **17**, 5096-5100(2006).
330. **Hui Pan***, Jizhong Luo, Han Sun, Yuan Ping Feng, Cheekok Poh, Jianyi Lin, Hydrogen Storage of ZnO and Mg Doped ZnO Nanowires, *Nanotechnology* **17**, 2963(2006).
331. **Hui Pan**, Yuan Ping Feng*, Jianyi Lin, *Ab Initio* Study of F, Cl-Functionalized Single Wall Carbon Nanotubes, *J. Phys.: Condens. Matter* **18**, 5175-5184(2006).
332. **Hui Pan***, Liying Tong, Yuan Ping Feng, Jianyi Lin, Enhancement of Minority-Carrier Lifetime by an Advanced High Temperature Annealing Method, *Thin Solid Films* **504**, 129-131 (2006).
333. **Hui Pan**, Jiabao Yi, Binghai. Liu, S. Thongmee, Jun Ding, Yuan Ping Feng, Jianyi Lin*, Magnetic Properties of Highly-Ordered Ni, Co and Their Alloy Nanowires in AAO Templates, *Solid State Phenomena* **111**, p123 (2006).
334. **Hui Pan**, Yuan Ping Feng*, Jianyi Lin, *Ab Initio* Study of Electronic and Optical Properties of Multiwall Carbon Nanotube Structures Made up of a Single Rolled-up Graphite Sheet, *Phys. Rev. B* **72**, 085415 (2005). Also highlighted on Virtual Journal of Nanoscale science & Technology 12 (7) (Aug. 15, 2005).
335. **Hui Pan**, Weizhe Chen, Sanhua Lim, Cheekoh Poh, Xiaobing Wu, Yuan Ping Feng, Wei Ji*, Jianyi Lin*, Photoluminescence and Optical Limiting of Si Nanowires, *J. Nanosci. Nanotechnol.* **5**, 733-737 (2005).
336. **Hui Pan**, Binghai Liu, Jiabao Yi, Cheekoh Poh, Sanhua Lim, Jun Ding, Yuan Ping Feng, Alfred Cheng Hon Huan, Jianyi Lin*, Growth of Single-Crystalline Ni and Co Nanowires via Electrochemical Deposition and Their Magnetic Properties, *J. Phys. Chem. B* **109**, 3094-3098 (2005).

337. **Hui Pan**, Yanwu Zhu, Zhenhua Ni, Han Sun, Cheekok Poh, Sanhua Lim, Chornghaur Sow, Zexiang Shen, Yuan Ping Feng, and Jianyi Lin*, Optical and Field Emission Properties of ZnO Nanostructures, *J. Nanosci. Nanotechnol.* **5**, 1683–1687 (2005).
338. **Hui Pan***, Han Sun, Cheekoh Poh, Yuan Ping Feng, Jianyi Lin, Single-crystal growth of metallic nanowires with preferred orientation, *Nanotechnology* **16**, 1559-1564 (2005).
339. **Hui Pan***, Sanhua Lim, Cheekoh Poh, Xiaobing Wu, Yuan Ping Feng, Jianyi Lin*, Growth of Si Nanowires by Thermal Evaporation, *Nanotechnology* **16**, 417-421 (2005).
340. **Hui Pan**, Yuan Ping Feng*, Jianyi Lin, *Ab Initio* Study of OH-Functionalized Single Wall Carbon Nanotubes, *Phys. Rev. B* **70**, 245425 (2004). Also highlighted on Virtual Journal of Nanoscale science & Technology 11 (1) (Jan. 10, 2005).
341. **Hui Pan***, Jianyi Lin, Yuan Ping Feng, Han Gao, Electrical Bridge Model on the Self-Organized Growth of Nanopores in Anodized Aluminum Oxide, *IEEE Trans. On Nanotechnology* **3**(4), 462-467 (2004).
342. **Hui Pan**, Han Gao, Sanhua Lim, Yuan Ping Feng, Jianyi Lin*, Highly Ordered Carbon Nanotubes Based on Porous Aluminum Oxide: Fabrication and Mechanism, *J. Nanosci. Nanotechnol.* **4** (8), 1014-1018 (2004).
343. Han Gao, Jianyi Lin*, **Hui Pan**, Guotao Wu, Yuan Ping Feng, The growth of Carbon Nanotubes at Predefined Locations Using Nickel Nanowires as Templates, *Chem. Phys. Lett.* **393**, 511 (2004).
344. **Pan Hui***, Cao Quanxi, Tong Liyin, Zhou Xiaohua, Applications of Carbon Nanotubes, *Micronanoelectronic Technology* **39**(9), 14-18 (2002). (in Chinese)
Pan Hui*, Tong Liyin, Cao Quanxi, Growth Mechanism of SiC Crystal by Sublimation, *Electronic Components & Materials* **21**(12), 17-19(2002). (in Chinese)

Book Chapters:

1. **Hui Pan**, Nanotubes for Energy Storage, “**Nanofabrication and its Application in Renewable Energy**”, edited by G. Zhang and N. Manjooran, The Royal Society of Chemistry 2014, pp. 120-197. (invited review)
2. **Hui Pan**, Progress on the Theoretical Study of Two-Dimensional MoS₂ Monolayer and Nanoribbon, “**MoS₂ – Materials, Physics, and Devices**”, edited by Z. M. Wang, Springer 2014, pp. 1-35. (invited review)
3. Yuan Ping Feng, **Hui Pan**, Rongqin Wu, Lei Shen, Jun Ding, Jiabao Yi, Yihong Wu, Ferromagnetism in Semiconductors Doped with Non-Magnetic Elements, “**Spintronics: Materials, Applications and Devices**”, edited by G. C. Lombardi and G. E. Bianchi, 2009, pp. 59-78. (invited review)
4. Jianyi Lin, **Hui Pan**, Yuan Ping Feng, Hydrogen Storage by Nanostructured Materials, “*Encyclopedia of Nanoscience and Nanotechnology*”, edited by Dr. H. S. Nalwa, American scientific Publisher, California 2011, pp. 225-253. (invited review)
5. Yuan Ping Feng, **Hui Pan**, Rongqin Wu, Guowen Peng, Jianyi Lin, *Ab Initio* study of Functionalized Nanotubes, “**Hard Nanomaterials**”, edited by Dr. H. S. Nalwa, 2006. (invited review)

International Conference/Workshop Talk List:

1. **Hui Pan**, Reconstruction Control for Improved Catalytic Activity. **Invited speaker**, International Conference on Materials for Advanced Technologies (ICMAT) 2025, Singapore, Jun. 29 – Jul. 04, 2025.
2. **Hui Pan**, Co-based tandem catalysts for enhanced nitrate electroreduction to ammonia. **Invited speaker**, International Conference on Materials for Advanced Technologies (ICMAT) 2025, Singapore, Jun. 29 – Jul. 04, 2025.
3. **Hui Pan**, In-Situ Reconstruction of Catalyst in Catalysis. **Invited speaker**, The 11th General Conference of the Asian Consortium on Computational Materials Science (ACCMS-11), Yokohama, Japan, May 31 – Jun. 3, 2025.
4. **Hui Pan**, Reconstruction Engineering for optimized catalytic performance. **Invited speaker**, The 2024 PKU International Forum on "AI +New Materials. Shenzhen, Dec. 3-5, 2024.
5. **Hui Pan**, 优化催化剂重构在催化反应中的应用. **Invited speaker**, 2024 年 NSFC-FDCT 前沿学科论坛—新时代材料科学高质量发展论坛, Guangxi, Nov. 29 – Dec. 1, 2024.
6. **Hui Pan**, 电解水产氢：催化剂的设计、制备及工业生产. **Invited speaker**, 2024 制氢电解槽耐久性技术与标准讨论会, Guangzhou, Nov. 22, 2024.
7. **Hui Pan**, In-Situ Reconstruction of Catalyst in Catalysis. **Invited speaker**, International Conference on Information Technology and Materials 2024, Hongkong, Nov. 8-11, 2024.
8. **Hui Pan**, Surface Reconstruction / Phase Transition in Catalysis. **Plenary Speaker**, 2024 Joint Annual Conference of Physical Societies in Guangdong-Hong Kong-Macao Greater Bay Area (YGA 2024), Macau, Jul. 29 – Aug. 01, 2024.
9. **Hui Pan**, Industrial Fabrication of Electrocatalysts for Green Hydrogen Production. **Keynote Speaker**, 2024 8th International Conference on Energy Technology and Materials Science (ICETMS 2024), Chongqing, May 17, 2024.
10. **Hui Pan**, Design and Industrial Fabrication of Electrocatalysts for Green Hydrogen Production. **Invited speaker**, The 6th International Symposium on Heat Transfer and Energy Conservation (ISHTEC2024), Guangzhou, Jan. 5-8, 2024.
11. **Hui Pan**, Electrocatalysts for Green Hydrogen Production - from Design to Industrial Fabrication. **Invited speaker**, International Conference on Materials for Advanced Technologies (ICMAT) 2023, Singapore, Jun. 26 -30, 2023.
12. **Hui Pan**, Green Hydrogen Production - Design and Fabrication of Electrocatalysts. **Invited Speaker**, Songshanhu Electrochemical Energy Conversion and Storage Materials Forum, Guangdong, May 12 – 15, 2023.
13. **Hui Pan**, Electrochemical Production of Green Hydrogen: from lab to industry. **Keynote talk**, the 4th international Conference on Advanced Materials and Clean Energy, Feb. 17, 2023.
14. **Hui Pan**, Electrocatalysts for Green Hydrogen Production: Design, Synthesis, and Industrial Fabrication, **Keynote talk**, The Asian Consortium on Computational Materials Science – Global Research Center (ACCMS-GRC), Webinar, Dec. 08, 2022.
15. **Hui Pan**, Electrocatalysts: Design, Fabrication, Industrial Production. **Invited talk**, International Conference of Green Energy and Catalysts, Huizhou, Nov. 19, 2022.
16. **Hui Pan**, Design of 2D materials for Nanodevices. **Invited talk**, 2022 International Conference on Low-Dimensional Semiconductor Materials and Device Physics, Chongqing, Nov. 19, 2022.
17. **Hui Pan**, Electrocatalysts: from Design, Fabrication to Industrial Production. **Invited talk**, 1st International Symposium on Advanced Functional Materials, Hangzhou, Nov. 14, 2022.
18. **Hui Pan**, Electrolysis of Water: Design, Fabrication to Industrial Production of Electrocatalysts. **Invited talk**, Zhejiang Technological University, Oct. 11, 2022.

19. **Hui Pan**, Water Electrolysis - Design, Fabrication to Industrial Production of Electrocatalysts. **Invited talk**, China South Normal University, Sep. 15, 2022.
20. **Hui Pan**, Electrolysis of Water: Design, Fabrication and Industrial Production of Electrocatalysts. **Invited talk**, Donghua University, Aug. 02, 2022.
21. **Hui Pan**, Design and Fabrication of Metal compounds for Electrolysis of Water, **Keynote talk**, 2022 International Conference on Energy Technology and Thermodynamic System (ETTS 2022). Jun. 24, 2022.
22. **Hui Pan**, Multi-metal compounds for Water Splitting, **Invited talk**, 闽澳学术论坛. May 19. 2022.
23. **Hui Pan**, Design and Fabrication of Materials for Multiple Applications – A view from “Solid State Physics”, **Invited talk**, Chongqing University, Mar. 24, 2022.
24. **Hui Pan**, Design and Fabrication of Electrocatalysts for Water Oxidization, **Keynote talk**, 2022 International Symposium on Green Energy Development Technology (GEDT 2022). Jan. 14, 2022.
25. **Hui Pan**, Design of Materials for Multi-functional Applications – A view from “Solid State Physics”, **Invited talk**, 5th Forum of Materials Genome Engineering (ForMGE), Zhengzhou, China, Dec. 15th -17th, 2021.
26. **Hui Pan**, Design of Materials for Multi-functional Applications, **Keynote talk**, 2021 5th International Conference on Sensors, Materials and Manufacturing (ICSMM 2021), 2021 5th International Conference on Advanced Manufacturing and Materials (ICAMM2021), and 2021 10th International Conference on Chemical Science and Engineering (ICCSE 2021), Nov. 19-21, 2021.
27. **Hui Pan**, Surface Reconstruction and Phase Transition of Electrocatalysts in OER, **Invited talk**, 1st International Conference on Energy Materials (ICEM) 2021, Nov. 5-8, 2021.
28. **Hui Pan**, Design of Catalysts for N₂-Reduction, **Invited talk**, Materials for Humanity (MH 21), Singapore, Jul. 6~9, 2021.
29. **Hui Pan**, P/N-Functionalized MXenes for Electrocatalysis, **Keynote talk**, IUMRS-ICA2020 & MRS-Thailand, Feb. 23-26, 2021.
30. **Hui Pan**, Enhanced Anchoring of Single-atom catalysts on N-functionalized MXenes for CO₂ reduction, **Invited talk**, The 3rd International Conference on MXenes, Ningbo, China, Oct. 11-14, 2020.
31. **Hui Pan**, Design and Fabrication of Nanomaterials for Energy Harvesting, **Keynote talk**, The 5th International Conference on Advances in Materials, Mechatronics and Civil Engineering (ICAMMCE 2020), Suzhou, China, Mar. 20-22, 2020.
32. **Hui Pan**, Design of Multi-functional 2D Materials, **Invited talk**, International Symposium on Condensed Matter Physics, Guangdong University, Nov. 09-10, 2019.
33. **Hui Pan**, Design of 2D Materials for Energy Harvesting, **Invited talk**, 粤港澳高校联盟 2019 年青年学者分论坛——基于超算先进材料应用研究, 中山大学国家超级计算广州中心, 2019/10/31.
34. **Hui Pan**, Design of Novel 2D Materials, **Invited talk**, the 10th International Conference of the Asian Consortium of Computational Materials Science (ACCMS-10), Hong Kong, Jul. 22-26, 2019.
35. **Hui Pan**, Design of co-catalysts for enhanced photocatalytic hydrogen production, **Invited talk**, The International Conference on Materials for Advanced Technologies (ICMAT) 2019, Singapore, Jun. 22~28, 2019.
36. **Hui Pan**, Design of 2D materials for multi-functional applications, **Invited talk**, The International Conference on Materials for Advanced Technologies (ICMAT) 2019, Singapore, Jun. 22~28, 2019.
37. **Hui Pan**, 2D Materials Design for Versatile Applications, **Invited talk**, the University of Electronic Science and Technology of China, Chengdu, China, June 14, 2019.
38. **Hui Pan**, Multifunctional applications of two-dimensional materials, **Invited talk**, Chongqing University, Chongqing, China, June 12, 2019.
39. **Hui Pan**, 2D Materials: From spintronics to catalysts, **Invited talk**, Chongqing University, Chongqing, China, June 11, 2019.
40. **Hui Pan**, Design of Pentagonal Monolayers for diverse applications, **Invited talk**, the 2nd International Conference on MXenes for Energy Applications, Beijing, China, May 10~12, 2019.

41. **Hui Pan**, Design of 2D materials for hydrogen production, **Invited Talk**, The 10th Singapore International Conference on Chemistry (SICC10), National University of Singapore, Singapore, Dec. 16-19, 2018.
42. **Hui Pan**, 2D materials as Electro-/Photo-catalysts, **Invited Talk**, The 8th Young Scholars Symposium on Nano & New Energy Technology (NNET 2018), Jinan University, Guangzhou, China, Sep. 26-29, 2018.
43. **Hui Pan**, Design of 2D monolayers as catalysts for energy harvesting, **Invited talk**, the Conference of the Asian Consortium on Computational Materials Science Theme Meeting (ACCMS-TM 2018), Ha Noi, Vietnam, Sep 6~9, 2018.
44. **Hui Pan**, Design and Fabrication of Catalysts for Water-Splitting, **Invited talk**, the 8th international conference on Advanced Functional Materials & Devices (AFMD), Catholic University of Leuven, Belgium, August 17~19, 2018.
45. **Hui Pan**, Hydrogen production from water, **Keynote talk**, the International Conference on Mechanical, Electric and Industrial Engineering (MEIE2018), Hangzhou, China, May 27~28, 2018.
46. **Hui Pan**, MXenes: Novel Catalysts for Hydrogen Production, **Invited talk**, the 1st International Conference on MXenes for Energy Applications, Changchun, China, May 25~26, 2018.
47. **Hui Pan**, Design and Fabrication of electrocatalysts for hydrogen production, **Invited Talk**, the South University of Science and Technology of China, Shenzhen on March 15-17, 2018.
48. **Hui Pan**, Materials Design for Solar-Driven Water Splitting, **Invited talk**, The 18th International Union of Materials Research Societies International Conference in Asia (IUMRS-ICA 2017), Taipei, Taiwan, Nov. 06~09, 2017.
49. **Hui Pan**, 2D Monolayers: Promising Materials for Versatile Applications, **Invited talk**, Huazhong University of Science and Technology, Wuhan, China, Aug. 03~06, 2017.
50. **Hui Pan**, Electronic, Magnetic, and Chemical Properties of 2D TMDs and MXenes, **Invited talk**, The 9th Joint Meeting of Chinese Physicists Worldwide (OCPA9), Beijing, China, Jul. 17~20, 2017.
51. **Hui Pan**, Electronic, Magnetic, and Chemical Properties of 2D Metal Nitrides and Phosphides, **Invited talk**, The International Conference on Materials for Advanced Technologies (ICMAT) 2017, Singapore, Jun. 18~23, 2017.
52. **Hui Pan**, Materials design for hydrogen production from water, **Plenary talk**, the 10th international conference on computational physics, Macao, Jan. 16~20, 2017.
53. **Hui Pan**, Multi-functional applications of 2D monolayers, **Invited Talk**, Zhejiang University of Technology, Hangzhou, on Oct. 10, 2016.
54. **Hui Pan**, Multi-functional applications of 2D monolayers, **Invited Talk**, Zhejiang University, Hangzhou, on Oct. 08, 2016.
55. **Hui Pan**, Materials design for solar energy harvesting, **Talk given**, South University of Science and Technology of China, Shenzhen on Aug. 08, 2016.
56. **Hui Pan**, Physical and Chemical Properties of Metal-dichalcogenides Monolayers, **Invited Talk**, The 2016 International Conference on Electronic Materials (ICEM2016), Jul. 4-8, 2016.
57. **Hui Pan**, Unique Electronic, Magnetic, and Chemical Properties of Metal-dichalcogenides Monolayers, **Talk given at the University of New South Wales, Sydney, Australia, on Jun. 17, 2016.**
58. **Hui Pan**, Electronic, Magnetic, and Chemical Properties of Metal-dichalcogenides Monolayers, **Talk given at the Institute of High Performance Computing, Singapore, on Feb. 12, 2016.**
59. **Hui Pan**, Waved Graphenes --- Unusual Physical and Chemical Properties, **Invited Talk**, **International Workshop on Functional Materials 2015 (Macau).**
60. **Hui Pan**, Unusual Mechanical, Electronic, Magnetic, and Chemical Properties of Waved Graphene. **The 4th Global Conference on Materials Science and Engineering Aug 3-6, 2015, Macau**
61. **Hui Pan**, Magnetic and Electronic Evolutions of Metal Dichalcogenide Monolayers Tuned by Hydrogenation and Strain. **The International Conference on Materials for Advanced Technologies 2015 (ICMAT2015), Singapore.**

62. **Hui Pan**, TiO₂-based photocatalyst for hydrogen production: dopant and defect, **Invited Talk, 2015 EMN East Meeting (Energy Material Nanotechnology), Apr. 20-23, Beijing (China)**.
63. **Hui Pan**, Electronic, Magnetic, and Catalytic properties of Transition Metal Dichalcogenide Monolayers, **Invited Talk, International Workshop on Functional Materials 2014 (Macau)**.
64. **Hui Pan**, Physical and Chemical Properties of 2D Metal Dichalcogenides, **Invited Talk, 2014 UM and HKU Joint Workshop on Science and Technology Innovation, 2014 (Macau)**.
65. **Hui Pan**, Design and Fabrication of TiO₂-based Photocatalyst for Hydrogen Production, **Invited Talk, Workshop on Functional Ceramics, University of Macau, 2013 (Macau SAR, China)**
66. **Hui Pan**, MoS₂ Nanoribbons: Effects of Edge and Strain on its Magnetic and Electronic Properties, **the 12th Asia-Pacific Physics Conference of AAPPS (APPC12) 2013 (Japan)**.
67. **Hui Pan**, Design of GaN-Based Photocatalyst for Hydrogen Production: ZnO-Codoped GaN Nanotubes, **the 7th International Conference on Materials for Advanced Technology (ICMAT) 2013 (Singapore)**.
68. **Hui Pan**, Edge-dependent Structural, Electronic, and Magnetic Properties of MoS₂ Nanoribbons, **The International Union of Materials Research Society – International Conference in Asia (IUMRS-ICA) 2012 (Korea)**.
69. **Hui Pan**, GaN/ZnO superlattice nanowires as photocatalyst for water-splitting: first-principles study on electronic and magnetic properties, **MRS Spring Meeting 2012 (USA)**.
70. **Hui Pan**, Effects of defects and (H, N)-codoping on the photocatalytic ability of TiO₂: a first-principles study, **MRS Spring Meeting 2011 (USA)**.
71. **Hui Pan** and Yong-Wei Zhang, ab initio study on the photocatalytic and magnetic properties of graphitic carbon nitride nanotubes, **MRS Spring Meeting 2011 (USA)**.
72. **Hui Pan**, Xiaofeng Qiu, Wenguan Zhu, Wei Wang, M. Parans Paranthaman, Gyula Eres, Zhenyu Zhang, Baohua Gu, Defect-Induced Bandgap Narrowing in TiO₂ and Photochemical Water Splitting in Visible Light, **MRS Fall Meeting 2008 (USA)**.
73. **Hui Pan**, Yuanping Feng, Jianyi Lin, Tungsten Carbide Nanotube for Hydrogen Adsorption: First-Principles Calculation, **AsiaNano 2008 (Singapore)**.
74. Yuan Ping Feng, **Hui Pan**, Jiabao Yi, Rongqin Wu, Lei Shen, Jun Ding, Jianyi Lin, Dilute Magnetic Semiconductors Without Magnetic Elements: First-Principles Prediction and Experimental Demonstration, **International Conference on Electronic Materials, IUMRS-ICEM 2008 (Australia)**.
75. **Hui Pan**, J Yi, J Y Lin, Y P Feng, J Ding, L H Van, J H Yin, Room Temperature Ferromagnetism in Carbon-Doped ZnO, **MRS Spring Meeting 2007 (USA)**.
76. **Hui Pan**, Yuanping Feng, Jianyi Lin, Magnetic Properties of OH-functionalized Carbon Nanotubes, **the 4th International Conference on Materials for Advanced Technologies (ICMAT) 2007 (Singapore)**.
77. **Hui Pan**, Rongqin Wu, Lei Shen, Jiabao Yi, Junhua Yang, Jianyi Lin, Yuan Ping Feng, Jun Ding, L H Van, J H Yin, Room Temperature Ferromagnetism in Carbon-Doped ZnO, **The 4th Conference of the Asian Consortium on Computational Materials Science 2007 (Korea)**.
78. **Hui Pan**, Jianyi Lin, Weizhe Chen, Han Sun, Yuanping Feng, Wei Ji, Optical Limiting and Hydrogen Storage Characterization of Cu, Cu₂O and CuO Nanostructures, **International Congress on Nanotechnology 2005 (USA)**.
79. **Hui Pan**, Zhenhua Ni, Han Sun, Cheekoh Poh, Zhexiang Shen, Yuanping Feng, Jianyi Lin, Optical and Raman Characterization of ZnO Nanowires, **The 3rd International Conference on Materials for Advanced Technologies (ICMAT) 2005 (Singapore)**.
80. **Hui Pan**, Quanxi Cao, Liyin Tong, Micro-defect in CZ-Si Crystal: its Control and Elimination, **The 8th International Conference on Electronic Materials 2002 (China)**

Member of Physical Society of Macau (PSM, Macau)
Member of Materials Research Society-Singapore (MRS-S)

Professional Services

- Co-general Chair of The 13th Asian Meeting on Ferroelectrics jointly with the 13th Asian Meeting on Electroceramics (AMF-13 & AMEC-13) November 12 – 16, 2023, Macau
- Member of Local Organizing Committee for the 10th Biennial International Conference of The Asian Consortium on Computational Materials Science (ACCMS-10), hosted by City University of Hong Kong for July 22 – 26, 2019.
- Member of International Advisory Committee in the 10th International Conference of Computational Physics (ICCP11). Hangzhou, China, Jun. 24-28, 2019.
- Session chair in the 10th International Conference on Materials for Advanced Technologies (ICMAT). Singapore, Jun. 23 - 28 2019.
- Session chair in the 2nd international conference on MXenes, Beijing, China, May 10-12, 2019.
- The Secretary of the 10th International Conference of Computational Physics (Macao, 2017)
- Chair of the symposium on “Computational Study on Nanosstructures” in the 10th international Conference on Computational Physics.
- Member of the Local Organizing Committee in the International Workshop on Solid-State Lighting of LED and Laser Diode, Macau 2016

Professional Review Services

Journals

Dr. Pan has served as a regular reviewer for more than 40 international SCI journals, such as Chemistry of Materials, ACS Nano, Physical Review B, Journal of Physical Chemistry, ACS Applied Materials & Interface, New Journal of Physics, Journal of Power Sources, Energy & Environmental Science, and Applied Catalyst B: Environmental.