

## Hui PAN (潘暉)

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Dr. Hui Pan is a professor in the Institute of Applied Physics and Materials Engineering and Founding Head of Department of Physics and Chemistry in the Faculty of Science and Technology 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 had 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 energy conversion and storage (such as electrocatalysis, photocatalysis, supercapacitors, hydrogen storage, and fuel cells), electronic devices, spintronics, and quantum devices. He has published more than **200** papers in international peer-reviewed journals, such as Phys. Rev. Lett., Phys. Rev. B, Adv. Energy Mater., Chem. Mater., ACS Nano, and J. Phys. Chem. B&C. The total citation is more than **9700** (**google scholar**) / **8100** (**SCI**). Additionally, he is the author of **5 book chapters** and the inventor of **4 USA** and **6 China** patents. His present h-index is **48** (**google scholar**) / **46** (**SCI**). (updated in Aug. 2021).

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## Education

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

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## Professional Experience

- Professor, University of Macau, Macau (August 2020 – present)
- Founding Head of Department of Physics and Chemistry, Faculty of Science and Technology, University of Macau, Macau (November 2018 - present)
- Associate Professor, University of Macau, Macau (August 2017 – August 2020)
- Assistant Professor, University of Macau, Macau (August 2013 – August 2017)
- Senior Scientist I, Institute of High Performance Computing, Singapore (April 2013 – August 2013)
- Scientist II, Institute of High Performance Computing, Singapore (April 2012 – March 2013)
- Scientist I, Institute of High Performance Computing, Singapore (May 2009 – March 2012)
- Postdoctoral Fellow, Oak Ridge National Laboratory, USA (April 2008 – April 2009)
- Research Fellow, National University of Singapore, Singapore (January 2006 – March 2008)

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## Teaching

### B.Sc. Courses

1. Physical Science – To know the natural laws around us

### PhD Courses

1. Solid State Physics
  2. Advanced Instrumentation for Materials Characterization
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## Research

### Research Interests

- Energy harvesting and storage (photocatalysis, electrocatalysis, CO<sub>2</sub> reduction, N<sub>2</sub> fixation, solar cell, fuel cell, hydrogen storage, and supercapacitor)
- Spintronics
- Nanodevices (ReRAM and PRAM)
- Fabrication and first-principles design of materials
- Condensed Matter Physics

### Research Grants

#### **Grants from Macau Government:**

- 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 (MYRG2017-00027-FST) (from 01/2018 to 12/2020)
- 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 (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: N23-2007/4

## Current Members

### *PhD and UG Students*

Mr. Ruchen Wu (PhD student, August 2021 ~ present)  
Ms. Lulu Qiao (PhD student, August 2021 ~ present)  
Ms. Lihong Yin (PhD student, August 2021 ~ present)  
Mr. Keyu An (PhD student, August 2021 ~ present)  
Mr. Xuanwei Dai (Undergraduate, October 2020 ~ present)  
Mr. Di Liu (PhD student, September 2020 ~ present)  
Mr. Haoyun Bai (PhD student, September 2020 ~ present)  
Mr. Jinxian Feng (PhD student, September 2020 ~ present)  
Mr. Bowen Li (PhD student, July 2020 ~ present)  
Mr. Pengfei Zhou (PhD student, July 2020 ~ present)  
Mr. Yunxiao Liu (Undergraduate, October 2019 ~ present)  
Mr. Mingpeng Chen (PhD student, August 2019 ~ present)  
Mr. Xinyu Du (PhD student, August 2019 ~ present)  
Mr. Haoqiang Ai (PhD student, August 2019 ~ present)  
Ms. Jiazhong Geng (PhD student, August 2019 ~ present)  
Ms. Feifei Li (PhD student, August 2019 ~ present)  
Ms. Zhiqin Ying (PhD student, August 2018 ~ present)  
Mr. Kin Long Ao (PhD student, August 2017 ~ present)

### *Research Staffs:*

Dr. Zhongbing PAN  
Dr. Yuyun CHEN  
Dr. Denny SIO  
Dr. Roger Yuanju QU  
Mr. Wenhao Gu  
Dr. Qingchun ZHANG  
Dr. Siying SHEN

## Former Members

### *PhD Graduates*

Dr. Yuanju Qu, Roger (PhD student from August 2014 to August 2017, graduated in August 2017)  
Dr. Ziqian Ma, Mason (PhD Student from August 2014 to April 2018, graduated in April 2018)  
Dr. Mengmeng Shao (PhD Student from August 2016 to May 2019, graduated in June 2019)  
Dr. Wenzhou Chen (PhD Student from August 2016 to May 2019, graduated in June 2019)  
Dr. Xiongwei Zhong (PhD Student from August 2016 to October 2019, graduated in October 2019)  
Dr. Lujie Cao (PhD Student from January 2016 to December 2019, graduated in January 2020)  
Dr. Mingyang Yang (PhD Student from January 2016 to December 2019, graduated in January 2020)  
Dr. Qing Zhu (PhD Student from August 2017 to June 2020, graduated in June 2020)  
Dr. Yangfan Shao (PhD Student from August 2016 to July 2020, graduated in August 2020)  
Dr. Rui Tong (PhD Student from August 2017 to July 2020, graduated in August 2020)  
Dr. Dong Liu (PhD student, January 2019 to July 2021, graduated in August 2021)  
Dr. Youchao Kong (PhD student, August 2018 to July 2021, graduated in August 2021)

### ***Undergraduates***

Mr. Shijie Wen, Jack (Undergraduate, graduated in 2016)  
Mr. Yifeng Xie (Undergraduate, graduated in 2018)  
Mr. Jialin Li (Undergraduate, graduated in 2018)  
Mr. Ye Ke (Undergraduate, graduated in 2018)  
Mr. Jer Shiuh Phoooh (Undergraduate, graduated in 2019)  
Ms. Ziqin Dai, Helen (Undergraduate, graduated in 2019)  
Ms. Ye Chen (Undergraduate, 06-07/2019)  
Mr. Shengjie Ding (Undergraduate, June 2018 ~ June 2020, graduated in 2020)

### ***Research Staffs***

Mr. Di Liu (currently PhD student in my Group)  
Dr. Zhen Li (@Shandong Normal University, Shandong, China)  
Dr. Chi Fong Wong (@City University of Macau)  
Dr. Tianwei He (@ Fritz Haber Institute of the Max Plank Society Berlin, Germany)  
Dr. Katherine Weng I Chio  
Dr. Pengcheng Zhao (@Northeast Petroleum University)  
Dr. Chao Peng (@WuYi University, Jiangmen, Guangdong, China)  
Mr. Ke-Yu An (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**, 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. 16/07/2021, **China Patent Application No. “submitted”**.
2. **Hui Pan**, Mingpeng Chen, and Bingpu Zhou, “2D MS<sub>2</sub> as Surface-enhanced Raman Scattering substrate for environmental and hygeian monitoring”, 16/07/2020, **China Patent Application No. “202010683464.2”**.
3. **Hui Pan**, Dong Liu and Guichuang Xing, “Bi-functional and low-cost elctrocatalyst for high-efficient and stable full-water-splitting: Cr-doped NiS<sub>x</sub>”, 16/08/2019, **China Patent Application No. “201910758027. X”**.
4. **Hui Pan** and Mengmeng Shao, “MoS<sub>2</sub>/Mo<sub>2</sub>C/CdS: a super-efficient photocatalyst for hydrogen evolution”, 21/11/2018, **China Patent Application No. “201811323293.1”**.
5. **Hui Pan** and Xiongwei Zhong, “Carbon-Coated N-rich C<sub>3</sub>N<sub>4</sub> as an anode material for Lithium Battery”, 12/02/2018, **Granted, China Patent No. ZL 201810148357.2**.
6. **Hui Pan** and Yuanju Qu, “TiS<sub>2</sub>: an excellent cathodic electrocatalyst for hydrogen production in electrolysis of water”, 26/09/2017, **Granted. China Patent No. ZL 201710917164.4**.
7. 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**.
8. **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**.
9. **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**.
10. **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. 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).
2. 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* (2021). (*Cover page article*)
3. Youchao Kong, Tianwei He\*, Alain R Puente Santiago, Dong Liu, Aijun Du, Shuangpeng Wang\*, and **Hui Pan\***, Unravelling the Reaction Mechanisms of N<sub>2</sub> Fixation on Molybdenum Nitride: A Full DFT study from the Pristine Surface to Heteroatom Anchoring. *ChemSusChem* (2021). (*Cover page article*)
4. 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* (2021).
5. 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* (2021).
6. 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* (2021). (*Cover page article*)
7. 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. Chem. Phys. Lett.* **12**, 6934-6940 (2021).
8. Chengqun Xu\*, Xiaolu Liu, Dezhi Li, Zeyuan Chen, Jiale Yang, Janjer Huang, and **Hui Pan\***, The coordination of  $\pi$ -delocalization in g-C<sub>3</sub>N<sub>4</sub> for efficient photocatalytic hydrogen evolution under visible light. *ACS Appl. Mater. Inter.* **13**, 20114–20124 (2021).
9. 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).
10. 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 – MSi<sub>2</sub>C<sub>x</sub>N<sub>4-x</sub> (M = Cr, Mo, and W; x = 1 and 2) - with tunable electronic and magnetic properties. *Nanoscale* **13**, 8038 - 8048 (2021). (*Cover Page Article*)
11. 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).
12. Jinxian Feng, Jun Ni and **Hui Pan\***, Synergistic Carbon and Hydrogen Reactions in Electrochemical Reduction of CO<sub>2</sub> to Liquid Fuels. *J. Mater. Chem. A* **9**, 10546 - 10561 (2021).
13. 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*)
14. 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<sub>x</sub>P for Enhanced Hydrogen Evolution Under Alkaline and Seawater Conditions by Promoting H<sub>2</sub>O Dissociation. *Small* **17**, 2007557 (2021).

15. 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*)
16. 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).
17. Feifei Li, Haoqiang Ai, Changmin Shi, Kin Ho Lo, and **Hui Pan\***, Single transition metal atom catalysts on Ti<sub>2</sub>CN<sub>2</sub> for efficient CO<sub>2</sub> reduction reaction. *Int. J. Hydro. Energy* **46**, 12886-12896 (2021).
18. 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<sub>1-x</sub>V<sub>x</sub>P nanoneedle arrays for hydrogen evolution reaction with large current density. *Science China Materials* **64**, 880-891(2021).
19. 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).
20. 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 MoSi<sub>2</sub>X<sub>4</sub> (X = N, P, and As). *Phys. Chem. Chem. Phys.* **23**, 3144 - 3151 (2021).
21. 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).
22. 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).
23. 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/Nb<sub>2</sub>O<sub>5</sub>@Nb<sub>2</sub>CT<sub>x</sub> (MXene) photocatalysts via steering charge kinetics strategy. *Chem. Eng. J.* **421**, 128766 (2021).
24. 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).
25. 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).
26. 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 BaTiO<sub>3</sub>-based Ceramics for Capacitor Applications. *Chemical Engineering Journal* **409**, 127375 (2021).
27. 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).
28. 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*)

29. 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).
30. 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).
31. 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)
32. 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).
33. Youchao Kong, Di Liu, Haoqiang Ai, Kin Ho Lo, Shuangpeng Wang\*, and **Hui Pan**\*, Theoretical Screening of Single Atoms Supported on Two-Dimensional Nb<sub>2</sub>CN<sub>2</sub> for Nitrogen Fixation. *ACS Appl. Nano Mater.* **3**, 11274–11281 (2020).
34. 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).
35. 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 MoOx/Ag/WOx as the Rear Transparent Electrode, *Adv. Mater. Interfaces* **7**, 2000591(2020).
36. Hui Zhang, Li-Ming Yang\*, **Hui Pan**, and Eric Ganz, Atomistic Level Mechanism of CO<sub>2</sub> Adsorption in N-ethylethylenediamine Functionalized M<sub>2</sub> (dobpdc) Metal–Organic Frameworks, *Crystal Growth & Design* **20**, 6337–6345 (2020).
37. 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).
38. Jinxian Feng and **Hui Pan**\*, Electronic State Optimization for Electrochemical N<sub>2</sub> Reduction Reaction in Aqueous Solution. *J. Mater. Chem. A* **8**, 13896 - 13915 (2020).
39. 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).
40. 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 MAPbI<sub>3</sub> Perovskite. *J. Mater. Chem. A* **8**, 13585-13593 (2020).
41. Jiazhong Geng, Iat-Neng Chan, Haoqiang Ai, Kin Ho Lo, Yoshiyuki Kawazoe, Kar Wei Ng\* and **Hui Pan**\*, Magnetic and electronic properties of 2D TiX<sub>3</sub> (X = F, Cl, Br and I). *Phys. Chem. Chem. Phys.* **22**, 17632 - 17638 (2020).
42. W. Chen, X. Chen, Y. Wu, G. Liu, and **Hui Pan**\*, First-principles investigation of ScX<sub>2</sub> (X= Cl, Br or I) monolayers for flexible spintronics and electronics. *Phys. Chem. Chem. Phys.* **22**, 14781-14786 (2020).
43. 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 Fe<sub>2</sub>TiO<sub>5</sub>/C hollow spheres as visible-light driven photocatalysts. *Mater. Design* **194**, 108928(2020).



44. Senchuan Huang, Yuying Meng\*, Yangfei Cao, Fen Yao, Zhujie He, Xuxu Wang, Hui Pan, and Mingmei Wu\*, Amorphous NiWO<sub>4</sub> nanoparticles boosting the alkaline hydrogen evolution performance of Ni<sub>3</sub>S<sub>2</sub> electrocatalysts. *Appl. Catal. B* **274**, 119120 (2020).
45. 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-MS<sub>2</sub> (M= Mo, W) nanosheets for surface-enhanced Raman scattering with long-term stability and large-scale uniformity. *Appl. Surf. Sci.* **527**, 146769 (2020).
46. **Hui Pan\***, Carrier-potential interaction for high-T<sub>c</sub> superconductivity. *Int. J. Mod. Phys. B* **34**, 2050163 (2020).
47. 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).
48. 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).
49. Haoqiang Ai, Youchao Kong, Di Liu, Feifei Li, Jiazhong Geng, Shuang-Peng Wang, Kin Ho Lo\* and **Hui Pan\***, 1T<sup>m</sup> Transition-Metal Dichalcogenides: Strong Bulk Photovoltaic Effect for Enhanced Solar-Power Harvesting. *J. Phys. Chem. C* **124**, 11221–11228 (2020).
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### **Book Chapters:**

1. **Hui Pan**, Nanotubes for Energy Storage, “**Nanofabrication and its Application in Renewable Energy**”, edited by G. Zhang and N. Manjooan, The Royal Society of Chemistry 2014, pp. 120-197. (invited review)
2. **Hui Pan**, Progress on the Theoretical Study of Two-Dimensional MoS<sub>2</sub> Monolayer and Nanoribbon, “**MoS<sub>2</sub> – 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**, Design of Catalysts for N<sub>2</sub>-Reduction, **Invited talk**, Materials for Humanity (MH 21), Singapore, Jul. 6~9, 2021.
2. **Hui Pan**, P/N-Functionalized MXenes for Electrocatalysis, **Keynote talk**, IUMRS-ICA2020 & MRS-Thailand, Feb. 23-26, 2021.
3. **Hui Pan**, Enhanced Anchoring of Single-atom catalysts on N-functionalized MXenes for CO<sub>2</sub> reduction, **Invited talk**, The 3<sup>rd</sup> International Conference on MXenes, Ningbo, China, Oct. 11-14, 2020.
4. **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.
5. **Hui Pan**, Design of Multi-functional 2D Materials, **Invited talk**, International Symposium on Condensed Matter Physics, Guangdong University, Nov. 09-10, 2019.
6. **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**.
7. **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.
8. **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.
9. **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.
10. **Hui Pan**, 2D Materials Design for Versatile Applications, **Invited talk**, the University of Electronic Science and Technology of China, Chengdu, China, June 14, 2019.
11. **Hui Pan**, Multifunctional applications of two-dimensional materials, **Invited talk**, Chongqing University, Chongqing, China, June 12, 2019.
12. **Hui Pan**, 2D Materials: From spintronics to catalysts, **Invited talk**, Chongqing University, Chongqing, China, June 11, 2019.
13. **Hui Pan**, Design of Pentagonal Monolayers for diverse applications, **Invited talk**, the 2<sup>nd</sup> International Conference on MXenes for Energy Applications, Beijing, China, May 10~12, 2019.
14. **Hui Pan**, Design of 2D materials for hydrogen production, **Invited Talk**, The 10<sup>th</sup> Singapore International Conference on Chemistry (SICC10), National University of Singapore, Singapore, Dec. 16-19, 2018.
15. **Hui Pan**, 2D materials as Electro-/Photo-catalysts, **Invited Talk**, The 8<sup>th</sup> Young Scholars Symposium on Nano & New Energy Technology (NNET 2018), Jinan University, Guangzhou, China, Sep. 26-29, 2018.
16. **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.
17. **Hui Pan**, Design and Fabrication of Catalysts for Water-Splitting, **Invited talk**, the 8<sup>th</sup> international conference on Advanced Functional Materials & Devices (AFMD), Catholic University of Leuven, Belgium, August 17~19, 2018.
18. **Hui Pan**, Hydrogen production from water, **Keynote talk**, the International Conference on Mechanical, Electric and Industrial Engineering (MEIE2018), Hangzhou, China, May 27~28, 2018.

19. **Hui Pan**, MXenes: Novel Catalysts for Hydrogen Production, **Invited talk**, the 1<sup>st</sup> International Conference on MXenes for Energy Applications, Changchun, China, May 25~26, 2018.
20. **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.
21. **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.
22. **Hui Pan**, 2D Monolayers: Promising Materials for Versatile Applications, **Invited talk**, Huazhong University of Science and Technology, Wuhan, China, Aug. 03~06, 2017.
23. **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.
24. **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.
25. **Hui Pan**, Materials design for hydrogen production from water, **Plenary talk**, the 10<sup>th</sup> international conference on computational physics, Macao, Jan. 16~20, 2017.
26. **Hui Pan**, Multi-functional applications of 2D monolayers, **Invited Talk**, Zhejiang University of Technology, Hangzhou, on Oct. 10, 2016.
27. **Hui Pan**, Multi-functional applications of 2D monolayers, **Invited Talk**, Zhejiang University, Hangzhou, on Oct. 08, 2016.
28. **Hui Pan**, Materials design for solar energy harvesting, **Talk given**, South University of Science and Technology of China, Shenzhen on Aug. 08, 2016.
29. **Hui Pan**, Physical and Chemical Properties of Metal-dichalcogenides Monolayers, **Invited Talk**, The 2016 International Conference on Electronic Materials (ICEM2016), Jul. 4-8, 2016.
30. **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.**
31. **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.**
32. **Hui Pan**, Waved Graphenes --- Unusual Physical and Chemical Properties, **Invited Talk, International Workshop on Functional Materials 2015 (Macau).**
33. **Hui Pan**, Unusual Mechanical, Electronic, Magnetic, and Chemical Properties of Waved Graphene. **The 4<sup>th</sup> Global Conference on Materials Science and Engineering Aug 3-6, 2015, Macau**
34. **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.**
35. **Hui Pan**, TiO<sub>2</sub>-based photocatalyst for hydrogen production: dopant and defect, **Invited Talk, 2015 EMN East Meeting (Energy Material Nanotechnology), Apr. 20-23, Beijing (China).**
36. **Hui Pan**, Electronic, Magnetic, and Catalytic properties of Transition Metal Dichalcogenide Monolayers, **Invited Talk, International Workshop on Functional Materials 2014 (Macau).**
37. **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).**
38. **Hui Pan**, Design and Fabrication of TiO<sub>2</sub>-based Photocatalyst for Hydrogen Production, **Invited Talk, Workshop on Functional Ceramics, University of Macau, 2013 (Macau SAR, China)**
39. **Hui Pan**, MoS<sub>2</sub> Nanoribbons: Effects of Edge and Strain on its Magnetic and Electronic Properties, **the 12<sup>th</sup> Asia-Pacific Physics Conference of AAPPS (APPC12) 2013 (Japan).**

40. **Hui Pan**, Design of GaN-Based Photocatalyst for Hydrogen Production: ZnO-Codoped GaN Nanotubes, **the 7<sup>th</sup> International Conference on Materials for Advanced Technology (ICMAT) 2013 (Singapore)**.
41. **Hui Pan**, Edge-dependent Structural, Electronic, and Magnetic Properties of MoS<sub>2</sub> Nanoribbons, **The International Union of Materials Research Society – International Conference in Asia (IUMRS-ICA) 2012 (Korea)**.
42. **Hui Pan**, GaN/ZnO superlattice nanowires as photocatalyst for water-splitting: first-principles study on electronic and magnetic properties, **MRS Spring Meeting 2012 (USA)**.
43. **Hui Pan**, Effects of defects and (H, N)-codoping on the photocatalytic ability of TiO<sub>2</sub>: a first-principles study, **MRS Spring Meeting 2011 (USA)**.
44. **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)**.
45. **Hui Pan**, Xiaofeng Qiu, Wenguan Zhu, Wei Wang, M. Parans Paranthaman, Gyula Eres, Zhenyu Zhang, Baohua Gu, Defect-Induced Bandgap Narrowing in TiO<sub>2</sub> and Photochemical Water Splitting in Visible Light, **MRS Fall Meeting 2008 (USA)**.
46. **Hui Pan**, Yuanping Feng, Jianyi Lin, Tungsten Carbide Nanotube for Hydrogen Adsorption: First-Principles Calculation, **AsiaNano 2008 (Singapore)**.
47. 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)**.
48. **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)**.
49. **Hui Pan**, Yuanping Feng, Jianyi Lin, Magnetic Properties of OH-functionalized Carbon Nanotubes, **the 4<sup>th</sup> International Conference on Materials for Advanced Technologies (ICMAT) 2007 (Singapore)**.
50. **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 4<sup>th</sup> Conference of the Asian Consortium on Computational Materials Science 2007 (Korea)**.
51. **Hui Pan**, Jianyi Lin, Weizhe Chen, Han Sun, Yuanping Feng, Wei Ji, Optical Limiting and Hydrogen Storage Characterization of Cu, Cu<sub>2</sub>O and CuO Nanostructures, **International Congress on Nanotechnology 2005 (USA)**.
52. **Hui Pan**, Zhenhua Ni, Han Sun, Cheekoh Poh, Zhexiang Shen, Yuanping Feng, Jianyi Lin, Optical and Raman Characterization of ZnO Nanowires, **The 3<sup>rd</sup> International Conference on Materials for Advanced Technologies (ICMAT) 2005 (Singapore)**.
53. **Hui Pan**, Quanxi Cao, Liyin Tong, Micro-defect in CZ-Si Crystal: its Control and Elimination, **The 8<sup>th</sup> International Conference on Electronic Materials 2002 (China)**

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#### Professional Affiliations

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

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#### Professional Services

- Member of Local Organizing Committee for the 10<sup>th</sup> 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 10<sup>th</sup> International Conference of Computational Physics (ICCP11). Hangzhou, China, Jun. 24-28, 2019.
- Session chair in the 10<sup>th</sup> International Conference on Materials for Advanced Technologies (ICMAT). Singapore, Jun. 23 - 28 2019.
- Session chair in the 2<sup>nd</sup> international conference on MXenes, Beijing, China, May 10-12, 2019.
- The Secretary of the 10<sup>th</sup> International Conference of Computational Physics (Macao, 2017)
- Chair of the symposium on “Computational Study on Nanosctructures” in the 10<sup>th</sup> 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.