

## Hui PAN (潘暉)

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Dr. Hui Pan is a full 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 and full professor in 2017 and 2020, respectively. 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 **170** papers in international peer-reviewed journals, such as Phys. Rev. Lett., Phys. Rev. B, Adv. Mater., Chem. Mater., ACS Nano, and J. Phys. Chem. B&C. The total citation is more than **8500 (google scholar) / 6970 (SCI)**. Additionally, he is the author of **5 book chapters** and the inventor of **4 USA** and **4 China** patents. His present h-index is **45 (google scholar) / 41 (SCI)**. (updated in Nov. 2020).

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## Education

- Ph.D. in Physics, National University of Singapore, Singapore (2006)
- B.Sc. in Electronic Materials and Devices, Xidian University, China (1997)

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## Professional Experience

- Professor, University of Macau, Macau (August 2020 – present)
- Founding Head 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) (1,997k MOP)
- Science and Technology Development Fund from Macao SAR (FDCT- 0154/2019/A3) (from 05/2020 to 05/2023) (2,410k MOP)
- Science and Technology Development Fund from Macao SAR (FDCT- 0102/2019/A2) (from 08/2019 to 07/2022) (2,590k MOP)
- Science and Technology Development Fund from Macao SAR (FDCT- 0035/2019/AGJ) (from 01/2020 to 12/2021) (1,120k MOP)
- Science and Technology Development Fund from Macao SAR (FDCT- 110/2014/SB) (from 11/2015 to 10/2018) (5,220k MOP)
- Science and Technology Development Fund from Macao SAR (FDCT-132/2014/A3) (from 06/2015 to 05/2018) (1,790k MOP)
- Science and Technology Development Fund from Macao SAR (FDCT-062/2014/A) (from 01/2015 to 12/2017) (790k MOP)
- Science and Technology Development Fund from Macao SAR (FDCT-076/2013/A) (from 01/2014 to 12/2014) (390k MOP)

#### Grants from University of Macau:

- Multi-year research grant at University of Macau (MYRG2017-00027-FST) (from 01/2018 to 12/2020) (897k MOP)
- Multi-year research grant at University of Macau (MYRG2018-00003-IAPME) (from 01/2019 to 12/2021) (899k MOP)
- Multi-year research grant at University of Macau (MYRG2015-00017-FST) (from 04/2015 to 09/2018) (1,300k MOP)
- Start-up research grant at University of Macau (SRG2013-00033-FST) (from 10/2013 to 09/2015) (100K MOP)
- Multi-year research grant at University of Macau (MYRG2014-000159-FST) (from 05/2014 to 04/2017) (500k MOP)

# Research Laboratory

Green Energy Materials Lab

## Current Members

### *PhD and UG Students*

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. Ke-Yu An (Research Assistant, July 2020 ~ present)  
Mr. Bowen Li (PhD student, July 2020 ~ present)  
Mr. Pengfei Zhou (PhD student, July 2020 ~ present)  
Mr. Youchao Kong (PhD student, October 2019 ~ present)  
Mr. Yunhao 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)  
Mr. Ye Ke (PhD student, August 2019 ~ present)  
Ms. Jiazhong Geng (PhD student, August 2019 ~ present)  
Ms. Feifei Li (PhD student, August 2019 ~ present)  
Mr. Dong Liu (PhD student, January 2019 ~ present)  
Mr. Yang Li (PhD student, August 2018 ~ present)  
Ms. Zhiqin Ying (PhD student, August 2018 ~ present)  
Mr. Kin Long Ao (PhD student, August 2017 ~ present)

### *Research Staffs:*

Dr. Yuyun Chen  
Dr. Zhen Li  
Dr. Pengcheng Zhao  
Dr. Denny Sio  
Mr. Ke-Yu An

## 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)

### *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 Shiu Phoo (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)

### **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**, Mingpeng Chen, and Bingpu Zhou, “2D MS<sub>2</sub> as Surface-enhanced Raman Scattering substrate for environmental and hygeian monitoring”, **China Patent Application No. “202010683464.2”**.
2. **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”**.
3. **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”**.
4. **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, **China Patent Application No. 201810148357.2**.
5. **Hui Pan** and Yuanju Qu, “TiS<sub>2</sub>: an excellent cathodic electrocatalyst for hydrogen production in electrolysis of water”, 26/09/2017, **China Patent Application No. 201710917164.4**.
6. 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**.
7. **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**.
8. **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**.
9. **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. Youchao Kong, Di Liu, Haoqiang Ai, Kin Ho Lo, Shuangpeng Wang\*, **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.* (2020).
2. 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* (2020).
3. 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* (2020).
4. 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* (2020).
5. 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.*, 2002464 (2020).
6. 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* (2020).
7. Chon Chio Leong, Yuanju Qu, Yoshiyuki Kawazoe, Sut Kam Ho, and **Hui Pan\***, MXenes: Novel Electrocatalysts for Hydrogen Production and Nitrogen Reduction. *Catal. Today*, (2020).
8. 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).
9. 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<sub>x</sub>/Ag/WO<sub>x</sub> as the Rear Transparent Electrode, *Adv. Mater. Interfaces*, 2000591(2020).
10. 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* (2020).
11. 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).
12. 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).
13. 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).
14. 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).

15. 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).
16. 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).
17. 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).
18. 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).
19. 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).
20. **Hui Pan**, Carrier-potential interaction for high-T<sub>c</sub> superconductivity. *Int. J. Mod. Phys. B* **34**, 2050163 (2020).
21. 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).
22. 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).
23. Haoqiang Ai, Youchao Kong, Di Liu, Feifei Li, Jiazhong Geng, Shuang-Peng Wang, Kin Ho Lo\* and **Hui Pan\***, 1T<sup>''</sup> Transition-Metal Dichalcogenides: Strong Bulk Photovoltaic Effect for Enhanced Solar-Power Harvesting. *J. Phys. Chem. C* **124**, 11221–11228 (2020).
24. 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).
25. 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<sub>x</sub>: Effects of Cr-doping and Phase Transition. *Appl. Catal. B* **267**, 118721 (2020).
26. 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).
27. 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).
28. 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-C<sub>3</sub>N<sub>4</sub>. *Int. J. Hydro. Energy* **45**, 18912-18921 (2020).
29. 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).
30. Lujie Cao, Yangfan Shao, **Hui Pan\*** and Zhouguang Lu\*, Designing Efficient Dual-Metal Single-Atom Electrocatalyst TMZn<sub>6</sub> (TM = Mn, Fe, Co, Ni, Cu, Zn) for Oxygen Reduction Reaction. *J. Phys. Chem. C* **124**, 11301-11307 (2020).

31. 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).
32. 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).
33. 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).
34. 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  $MoS_2$  with  $Ni_5P_4$ - $Ni_2P$  Template. *J. Electrochem. Soc.* **167**, 026511 (2020).
35. 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  $Co_3O_4$  and Nitrogen-Doped Active Carbon toward Bifunctional Catalyst for Zinc-Air Batteries, *Appl. Catal. B* **260**, 118188 (2020).
36. Tianqi Deng, Yong Xue, Wen Shi, Zicong Marvin Wong, Gang Wu, **Hui Pan**, Jian-Sheng Wang, and Shuo-Wang Yang\*, Beyond Mahan-Sofo Best Thermoelectric Strategy: High Thermoelectric Performance from Directional  $\pi$ -Conjugation in Two-Dimensional Poly (tetrathienoanthracene). *J. Mater. Chem. A* **8**, 4257-4262 (2020).
37. 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  $B_4Al_n^{0/-/+}$  (n= 1-5). *Mater. Today Commun.* **24**, 100914 (2020).
38. 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).
39. 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).
40. 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- $C_3N_4$ , *J. Phys. Chem. C* **123**, 26136-26144 (2019).
41. 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).
42. 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).
43. Feifei Li, Li Chen, Hongmei Liu, Dongchao Wang, Changmin Shi\* and **Hui Pan\***, Enhanced  $N_2$ -fixation by Engineering the Edges of Two-dimensional Transition Metal Disulfides, *J. Phys. Chem. C* **123**, 22221-22227 (2019).
44. 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).
45. Shu Hearn Yu, Zhe Tang, Yangfan Shao, Haiwen Dai, Hong Yu Wang, Jiixin Yan, **Hui Pan**, and Daniel H. C. Chua\*, In-situ hybridizing  $MoS_2$  microflowers on  $VS_2$  microflakes in a one-pot



- CVD process for electrolytic hydrogen evolution reaction. *ACS Appl. Energy Mater.* **2**, 5799-5808 (2019).
46. 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  $\beta$ -AuSe with multiple superior properties: a first-principles investigation. *J. Phys. Condens. Matter* **31**, 395501 (2019).
  47. Mengmeng Shao, Wenzhou Chen, Shengjie Ding, Kin Ho Lo, Xiongwei Zhong, Linmin Yao, Weng Fai Ip, Baomin Xu, Xuesen Wang, and **Hui Pan\***,  $WX_y/g$ - $C_3N_4$  ( $X = C, N \& S$ ) composites for highly efficient photocatalytic water splitting, *ChemSusChem* **12**, 3355 – 3362 (2019).
  48. Yangfan Shao, Penglai Gong, **Hui Pan\***, and Xingqiang Shi\*, H-/dT-MoS<sub>2</sub>-on-MXene Heterostructures as Promising 2D Anode Materials for Lithium-Ion Batteries: Insights from First-Principles. *Advanced Theory and Simulations* **2**, 1900045 (2019).
  49. Mingyang Yang, Xuelian Fu, Jianqiao Zhang, Zhenyu Wang, Bingxue Wang, Liqing He, Zhiliang Wu, Hua Cheng, **Hui Pan\***, and Zhouguang Lu\*, Hierarchical Ultrafine Ni<sub>3</sub>V<sub>2</sub>O<sub>8</sub> Nanoparticles Anchored on rGO as High-Performance Anode Materials for Lithium-Ion Batteries, *Energy Technology* **7**, 1800784 (2019).
  50. 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).
  51. 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).
  52. Qing Zhu, Wenzhou Chen, Hua Cheng, Zhouguang Lu, and **Hui Pan\***, WS<sub>2</sub> Nanosheets with Highly-Enhanced Electrochemical Activity by Facile Control of Sulphur Vacancies. *ChemCatChem* **11**, 2667-2675 (2019).
  53. Yangfan Shao, Qian Wang, Liang Hu, **Hui Pan\***, and Xingqiang Shi\*, BC<sub>2</sub>N monolayer as a promising anchoring material for lithium-sulfur batteries: a first-principles study. *Carbon* **149**, 530-537 (2019).
  54. 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).
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**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. 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 Novel 2D Materials, **Invited talk** given at the 10th International Conference of the Asian Consortium of Computational Materials Science (ACCMS-10), Hong Kong, Jul. 22-26, 2019.
2. **Hui Pan**, Design of co-catalysts for enhanced photocatalytic hydrogen production, **Invited talk** given at The International Conference on Materials for Advanced Technologies (ICMAT) 2019, Singapore, Jun. 22~28, 2019
3. **Hui Pan**, Design of 2D materials for multi-functional applications, **Invited talk** given at The International Conference on Materials for Advanced Technologies (ICMAT) 2019, Singapore, Jun. 22~28, 2019
4. **Hui Pan**, 2D Materials Design for Versatile Applications, **Invited talk** at the University of Electronic Science and Technology of China, Chengdu, China, June 14, 2019.
5. **Hui Pan**, Multifunctional applications of two-dimensional materials, **Invited talk** at Chongqing University, Chongqing, China, June 12, 2019.
6. **Hui Pan**, 2D Materials: From spintronics to catalysts, **Invited talk** at Chongqing University, Chongqing, China, June 11, 2019.
7. **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.
8. **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.
9. **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.
10. **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.
11. **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.
12. **Hui Pan**, Hydrogen production from water, **Keynote talk**, the International Conference on Mechanical, Electric and Industrial Engineering (MEIE2018), Hangzhou, China, May 27~28, 2018.
13. **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.
14. **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.
15. **Hui Pan**, Materials Design for Solar-Driven Water Splitting, **Invited talk given at The 18th International Union of Materials Research Societies International Conference in Asia (IUMRS-ICA 2017), Taipei, Taiwan, Nov. 06~09, 2017**
16. **Hui Pan**, 2D Monolayers: Promising Materials for Versatile Applications, **Invited talk given at Huazhong University of Science and Technology, Wuhan, China, Aug. 03~06, 2017**
17. **Hui Pan**, Electronic, Magnetic, and Chemical Properties of 2D TMDs and MXenes, **Invited talk given at The 9th Joint Meeting of Chinese Physicists Worldwide (OCPA9), Beijing, China, Jul. 17~20, 2017**
18. **Hui Pan**, Electronic, Magnetic, and Chemical Properties of 2D Metal Nitrides and Phosphides, **Invited talk given at The International Conference on Materials for Advanced Technologies (ICMAT) 2017, Singapore, Jun. 18~23, 2017**

19. **Hui Pan**, Materials design for hydrogen production from water, **Plenary talk given at the 10<sup>th</sup> international conference on computational physics, Macao, Jan. 16~20, 2017**
20. **Hui Pan**, Multi-functional applications of 2D monolayers, **Invited Talk given at Zhejiang University of Technology, Hangzhou, on Oct. 10, 2016.**
21. **Hui Pan**, Multi-functional applications of 2D monolayers, **Invited Talk given at Zhejiang University, Hangzhou, on Oct. 08, 2016.**
22. **Hui Pan**, Materials design for solar energy harvesting, **Talk given at the South University of Science and Technology of China, Shenzhen on Aug. 08, 2016.**
23. **Hui Pan**, Physical and Chemical Properties of Metal-dichalcogenides Monolayers, **Invited Talk, The 2016 International Conference on Electronic Materials (ICEM2016), Jul. 4-8, 2016.**
24. **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.**
25. **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.**
26. **Hui Pan**, Waved Graphenes --- Unusual Physical and Chemical Properties, **Invited Talk, International Workshop on Functional Materials 2015 (Macau).**
27. **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**
28. **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.**
29. **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).**
30. **Hui Pan**, Electronic, Magnetic, and Catalytic properties of Transition Metal Dichalcogenide Monolayers, **Invited Talk, International Workshop on Functional Materials 2014 (Macau).**
31. **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).**
32. **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)**
33. **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).**
34. **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).**
35. **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).**
36. **Hui Pan**, GaN/ZnO superlattice nanowires as photocatalyst for water-splitting: first-principles study on electronic and magnetic properties, **MRS Spring Meeting 2012 (USA).**
37. **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).**
38. **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).**
39. **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).**
40. **Hui Pan**, Yuanping Feng, Jianyi Lin, Tungsten Carbide Nanotube for Hydrogen Adsorption: First-Principles Calculation, **AsiaNano 2008 (Singapore).**

41. 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)*.
42. **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)*.
43. **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)*.
44. **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)*.
45. **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)*.
46. **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)*.
47. **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.