

Selected publications (*Corresponding Author)

1. 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*, **2106091** (2022).
2. 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).
3. 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).
4. 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).
5. 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*)
6. 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*)
7. 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).
8. 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*)
9. 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).
10. 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).
11. 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*)

12. 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).
13. 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).
14. 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*)
15. 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).
16. 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).
17. 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).
18. 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).
19. 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).
20. 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).
21. 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).
22. 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*)
23. 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).
24. 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).
25. Jinxian Feng and **Hui Pan***, Electronic State Optimization for Electrochemical N₂ Reduction Reaction in Aqueous Solution. *J. Mater. Chem. A* **8**, 13896 - 13915 (2020).
 26. 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).
 27. **Hui Pan***, Carrier-potential interaction for high-T_c superconductivity. *Int. J. Mod. Phys. B* **34**, 2050163 (2020).
 28. 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).
 29. Haoqiang Ai, Youchao Kong, Di Liu, Feifei Li, Jiazhong Geng, Shuang-Peng Wang, Kin Ho Lo* and **Hui Pan***, 1T^m Transition-Metal Dichalcogenides: Strong Bulk Photovoltaic Effect for Enhanced Solar-Power Harvesting. *J. Phys. Chem. C* **124**, 11221–11228 (2020).
 30. 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).
 31. 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).
 32. **Hui Pan***, Carrier-potential interaction for high-T_c superconductivity. *Int. J. Mod. Phys. B* **34**, 2050163 (2020).
 33. 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).
 34. 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).
 35. 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.**
 36. 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).
 37. 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).
 38. 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.**
39. 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).
 40. 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).
 41. 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).
 42. 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 $V_2O_5@Ni_3S_2$ hybrid nanoarray for pseudocapacitors and hydrogen production. *J. Mater. Chem. A* **5**, 17954 – 17962 (2017).
 43. 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 Ti_2C and g- C_3N_4 for efficient photocatalytic hydrogen production. *J. Mater. Chem. A*, **5**, 16748–16756 (2017).
 44. 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 VS_2 nanoflowers for efficient hydrogen evolution reaction. *J. Mater. Chem. A* **5**, 15080 - 15086 (2017).
 45. 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 Ni_3S_2 Nanowire Arrays as Active Electrocatalyst for Hydrogen Evolution Reaction. *ACS Appl. Mater. Interfaces* **9**, 5959–5967 (2017).
 46. **Hui Pan***, Ultra high electrochemical catalytic activity of MXenes. *Scientific Reports* **6**, 32531 (2016).
 47. **Hui Pan***, Principles on design and fabrication of nanomaterials as photocatalyst for water-splitting. *Renew. Sustain. Energy Rev.* **57**, 584–601 (2016).
 48. **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.**
 49. Yuanju Qu, **Hui Pan***, Chi Tat Kwok, and Zisheng Wang, A First-Principles Study on Hydrogen Evolution Reaction of VS_2 Nanoribbons. *Phys. Chem. Chem. Phys.* **17**, 24820–24825 (2015).
 50. **Hui Pan***, Magnetic and electronic evolutions of hydrogenated VTe_2 monolayer under tension. *Scientific Reports* **4**, 7524 (2014).
 51. **Hui Pan***, Metal dichalcogenides monolayers: Novel catalysts for electrochemical hydrogen production, *Scientific Reports* **4**, 5348 (2014).
 52. **Hui Pan*** and Bin Chen, Ultra-flexibility and unusual electronic, magnetic, and chemical properties of waved graphenes and nanoribbons, *Scientific Reports.* **4**, 4198 (2014).
 53. **Hui Pan***, Electronic and magnetic properties of vanadium dichalcogenides monolayers tuned by hydrogenation, *J. Phys. Chem. C* **118**, 13248–13253 (2014).

54. **Hui Pan***, Jianyi Lin, Yuan Ping Feng, Carbon Nanotubes for Supercapacitor, *Nanoscale Res. Lett.* **5**, 654-668 (2010) (review).
55. **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).
56. **Hui Pan**, Yuan Ping Feng*, Semiconductor Nanowires and Nanotubes: Effects of Size and Surface-to-Volume Ratio, *ACS Nano* **2**, 2410-2414 (2008).
57. **Hui Pan***, Cheekok Poh, Yuan Ping Feng, Jianyi Lin*, Supercapacitor Electrodes from Tubes-in-Tube Carbon Nanostructures, *Chem. Mater.* **19**, 6120 (2007).
58. **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)*).
59. **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).