

Yulan Han

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Education

- 2020 – 2024 **Ph.D. in Chemistry**, School of Chemistry and Chemical Engineering, Queen's University Belfast, UK
- 2017-2020 **M.S. in Physical Chemistry**, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Anhui, China
- 2013-2017 **B.S. in Chemistry**, Department of Science, China University of petroleum, Qingdao, China

Research Experience

- Aug.2024 – Now **Postdoc**, Department of Chemistry and Biochemistry, University of California, Los Angeles
Advisor: Prof. Anastassia Alexandrova
- 2020 – 2024 **Ph.D. student**, School of Chemistry and Chemical Engineering, Queen's University Belfast, UK
Advisor: Prof. Peijun Hu (Elected Member of Royal Irish Academy)
Conducted operando modeling of syngas reactions on a metal oxide-zeolite (OX-ZEO) bifunctional catalyst to elucidate surface reconstruction phenomena under realistic reaction conditions and explored the structure-activity relationships via an integrated machine learning-accelerated techniques (Genetic Algorithm/Monte Carlo/Molecular Dynamics).
- 2017 – 2020 **M.S. Student**, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Anhui, China
Advisor: Prof. Jun Jiang & Dr. Guozhen Zhang
Conducted a comprehensive investigation into the influence of interlayer and intralayer single atom models on oxygen reduction reactions under controlled conditions of constant charge and constant potential.
- 2016 – 2017 **Undergraduate research**, Department of Science, China University of petroleum, Qingdao, China
Advisor: Dr. Hui Fu
Studied the effect of exchanged zeolite on the cracking of butene.

Publication

Total citations: 525 ([Google Scholar](#), Nov 2023); # = co-first authorship.

13. **Han, Y.**[#]; Xu, J.[#]; Xie, W.; Wang, Z.; Hu, P., Unravelling the Impact of Metal Dopants and Oxygen Vacancies on Syngas Conversion over Oxides: A Machine Learning-Accelerated Study of CO Activation on Cr-Doped ZnO Surfaces. *ACS Catal.* **2023**, 13, 15074–15086. (IF = 13.7, citation = 0)

12. **Han, Y.**[#]; Ye, K.[#]; Huang, Y.; Wu, Z.; Hu, P.; Zhang, G., Leveraging interlayer interaction in M-N-C catalysts for enhanced activity in oxygen reduction reactions. *J. Phys. Chem. Lett.* **2023**, 14, 44, 9900–9908. (IF = 6.9, citation = 0)
11. **Han, Y.**; Xu, J.; Xie, W.; Wang, Z.; Hu, P., Comprehensive Study of Oxygen Vacancies on the Catalytic Performance of ZnO for CO/H₂ Activation Using Machine Learning-Accelerated First-Principles Simulations. *ACS Catal.* **2023**, 13, 5104-5113. (IF = 13.7, citation = 4)
10. **Han, Y.**[#]; Li, Q.-K.[#]; Ye, K.; Luo, Y.; Jiang, J.; Zhang, G., Impact of active site density on oxygen reduction reactions using monodispersed Fe–N–C single-atom catalysts. *ACS Appl. Mater. Interfaces* **2020**, 12 (13), 15271-15278. (IF = 10.4, citation = 50)
9. Qian, Y.[#]; **Han, Y.**[#]; Zhang, X.; Yang, G.; Zhang, G.; Jiang, H.-L., Computation-Based Regulation of Excitonic Effects in Donor-Acceptor Covalent Organic Frameworks for Enhanced Photocatalysis. *Nat. Commun.* **2023**, 14, 3083 (IF = 17.7, citation = 16)
8. Zhang, K.[#]; **Han, Y.**[#]; Qiu, J.; Ding, X.; Deng, Y.; Wu, Y.; Zhang, G.; Yan, L., Interface engineering of Ni/NiO heterostructures with abundant catalytic active sites for enhanced methanol oxidation electrocatalysis. *J. Colloid Interface Sci.* **2023**, 630, 570-579. (IF = 10.0, citation = 18)
7. Qiu, J.[#]; **Han, Y.**[#]; Zhang K.; Deng Y.; Wu Y.; Yan L., 3D Pt/2D-NiMOF/rGO-Supported Subsized Pt Nanoparticles for Excellent CO Tolerance and Improved Methanol Oxidation in Both Alkaline and Acidic Media. *ACS Appl. Energy Mater.* **2022**, 5(4), 4439-4447. (IF = 7.0, citation = 6)
6. Wei, C.[#]; **Han, Y.**[#]; Liu, H.; Gan, R.; Ma, W.; Liu, H.; Song, Y.; Zhang, X.; Shi, J.; Ma, C., Enhancing conversion of polysulfides via porous carbon nanofiber interlayer with dual-active sites for lithium-sulfur batteries. *J. Colloid Interface Sci.* **2022**, 625, 946-955. (IF = 10.0, citation = 4)
5. Wei, C.[#]; **Han, Y.**[#]; Liu, H.; Gan, R.; Li, Q.; Wang, Y.; Hu, P.; Ma, C.; Shi, J., Advanced lithium–sulfur batteries enabled by a SnS₂-Hollow carbon nanofibers Flexible Electrocatalytic Membrane. *Carbon* **2021**, 184, 1-11. (IF = 11.3, citation = 22)
4. Wang, Z.[#]; **Han, Y.**[#]; Liang, J.; Huang, H.; Hu, C.; Liu, P.; Xiang, J.; Qi, Z.; Lu, Y.; Liu, K., Hydrogenation-Induced Phase Transition in Atomic-Layered α -MoCl₃ Driven by Laser Illumination in a Moist Atmosphere. *ACS Appl. Electron. Mater.* **2020**, 2 (8), 2678-2684. (IF = 4.5, citation = 3)
3. Wang, Z.[#]; **Han, Y.**[#]; Liu, P.; Li, Y.; Xu, S.; Xiang, J.; Ali, R. N.; Su, F.; Zeng, H.; Jiang, J., Electronic transport and optoelectronic applications of a new layered semiconductor CuTaS₃. *Appl. Surf. Sci.* **2020**, 499, 143932. (IF = 7.4, citation = 8)
2. Li, J.[#]; **Han, Y.**[#]; Ji, T.; Wu, N.; Lin, H.; Jiang, J.; Zhu, J., Porous metallosalen hypercrosslinked ionic polymers for cooperative CO₂ cycloaddition conversion. *Ind. Eng. Chem. Res.* **2019**, 59 (2), 676-684. (IF = 4.3, citation = 31)
1. Li, J.[#]; **Han, Y.**[#]; Lin, H.; Wu, N.; Li, Q.; Jiang, J.; Zhu, J., Cobalt–salen-based porous ionic polymer: the role of valence on cooperative conversion of CO₂ to cyclic carbonate. *ACS Appl. Mater. Interfaces* **2019**, 12 (1), 609-618. ((IF = 10.4, citation = 48)

Awards

- 2023 Scholarship from the European Union's Horizon 2020 research and innovation program, Queen's University Belfast, UK
- 2020 China Scholarship Council (CSC) scholarships, Queen's University Belfast, UK
- 2020 Queen's University Belfast Full Tuition Fee scholarship, Queen's University Belfast, UK
- 2017-2020 The First-order Academic Scholarship (3 times), University of Science and Technology of China, Anhui, China
- 2017 Second Prize, Hefei National Research Center for Microscale Physical Sciences Graduate Special Scholarship, University of Science and Technology of China, Anhui, China
- 2014-2016 National Encouragement Scholarship (3 times), China University of petroleum, Qingdao, China

Invited Talk

- 2023.04 "Exploration of Active Phases in $Zn_xCr_yO_z$ ", Annual Conference on Theoretical Catalytic Conversion of Carbon-Based Small Molecules, Xiamen University.
- 2023.11 "A Machine Learning-Accelerated Study of CO Activation on Cr-Doped ZnO Surfaces", Annual Conference on Theoretical Catalytic Conversion of Carbon-Based Small Molecules, ShanghaiTech University.

Research Mentoring

Yue Yang, Ph.D. Student (School of Chemistry and Molecular Engineering), (2021 – present)
EUSTC

Qianyun Wu, M.S. Student (School of Chemistry and Molecular Engineering), (2021 – present)
EUSTC