Wenqiang Yang

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Department of Chemical Engineering
University of South Carolina
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EDUCATION

University of South Carolina Columbia, United States
Ph.D. in Chemical Engineering, 08/2015 – 08/2020
Thesis: "Theoretical Investigation of the Biomass Conversion on Transition Metal Surfaces Based on Density Functional Theory Calculations and Machine Learning"

University of Science and Technology of China Hefei, China
Master in Material Science and Engineering, 09/2012 – 06/2015
Thesis: "A First Principle's Study of the Performance Improvement of the $La_{1-x}Sr_xCo_{1-y}Fe_yO_{3-\delta}$ Cathode in Solid Oxide Fuel Cells"

Nanjing University of Science and Technology Nanjing, China
Bachelor of engineering in Material Science and Engineering, 09/2008 – 06/2012

RESEARCH EXPERIENCE

University of South Carolina, Columbia, US *09/2023 – present*
Research assistant professor, department of Chemical Engineering

- Catalysts for liquid organic hydrogen carriers for hydrogen storage.
- CO_2 capture materials for CO_2 emission reduction and usage.
- Solvent effect in heterogenous catalysis, such as hydrogen evolution reaction.

Technical University of Denmark, Lyngby, Denmark *07/2021 – 07/2023*
Postdoctoral Fellow, department of Physics, CatTheory Center

- Machine learning prediction of the oxygen species adsorption on metal oxide surfaces.
- The inverse design problem in heterogeneous catalysis and its application in CO methanation over Ni_xFe_y metal alloy catalysts.
- The spin effect of metal dopants on Ni catalyzed CO methanation reactions.

University of South Carolina, Columbia, US *05/2020 – 06/2021*
Postdoctoral Fellow, department of Chemical Engineering

- Rational design of transition metal catalysts for the hydrodeoxygenation of succinic acid based on machine learning and microkinetic modelling.
- Develop microkinetic model to identify reaction mechanisms, rate-controlling steps and key intermediates under various reaction conditions.
- Identify correlations between activity (selectivity) and machine learning identified descriptors.

Graduate Student, department of Chemical Engineering

- Investigate the hydrodeoxygenation (HDO) of propanoic acid (Pac) on transition metal surfaces.

- Built machine learning models to predict the adsorption energy and transition states that involved in the HDO of Pac over 8 transition metal surfaces.
- Calculate the descriptor values for all possible catalysts and to find the optimal catalyst with high activity and selectivity to specific products.

University of Science and Technology of China, Hefei, China 09/2012-06/2015

Master Student, Department of Materials Science and Engineering

- Exploring mechanisms underlying the enhanced performance of Pt infiltrated $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (LSCF) cathode in solid oxide fuel cells (SOFCs).
- Investigating the steam reforming over SOFCs' anode (Ni/TiO2) via first principle's calculations.

PUBLICATIONS

Total publication to present: 30; Total citation: 649; H-index: 14

1. R. Zou, W. Yang, B. Rezaei, K. Tang, K. Guo, P. Zhang, S. S. Keller, H. R. Andersen, Y. Zhang, Activation of peracetic acid by electrodes using biogenic electrons: A novel energy- and catalyst-free process to eliminate pharmaceuticals. *Water Research*, **2024**, 261, 122065.
2. W. Yang, Z. Wang, and J. K. Nørskov, CO Methanation over Ni−Fe Alloy Catalysts: An Inverse Design Problem. *ACS catalysis*, **2024**, 14, 11657-11665.
3. W. Yang, K. E. Abdelfatah, S. K. Kundu, B. Rajbanshi, G. A. Terejanu, A. Heyden, Machine learning accelerated first principles study of the hydrodeoxygenation of propanoic. *ACS catalysis*, **2024**, 14, 10148-10163.
4. X. Xie, C. Li, Z. Lu, Y. Wang, W. Yang, M. Chen, W. Li, Noble metal modified copper-exchanged mordenite zeolite (Cu-ex-MOR) catalysts for catalyzing the methane efficient gas-phase synthesis methanol. *Energy*, **2024**, 300, 131595.
5. C. Kong, C. Zhi, Z. Wu, W. Yang, J. Yang, Z. Sun, Tailoring hypervalent Nickel induced by oxygen vacancy toward enhanced oxygen evolution reaction performance in self-supporting NiFe-(oxy) hydroxides electrodes. *Journal of Colloid And Interface Science*, **2024**, 665, 863–870.
6. D. Hui, C. Ye*, X. Cao, Y. Hu, S. Chen, W. Yang*, L. Hu*, G. Pan*, Unraveling the Molecular Weight Dependence of High Magnetic Field to Manipulate the Semiconducting Polymer Molecular Orientation. *ACS Appl. Mater. Interfaces*, **2024**, 16, 19, 25013–25024. ***(*Co-corresponding author)***
7. H. Zhao, Q. Yang, D. Zhu*, W. Yang*, Z. Shi , X. Li, Y. Ding, W. Guo, J. Gu, Y. Song *, J. Sun*, Cooperative Co single atoms and Co_2P nanoparticles as catalytic tandem for boosting redox kinetics in LieS batteries. *Materials Today Energy*, **2024**, 40, 101504. ***(*Co-corresponding author)***
8. R. Zou, W. Yang, B. Rezaei, K. Tang, P. Zhang, H. R. Andersen, S. S. Keller, Y. Zhang, Sustainable bioelectric activation of periodate for highly efficient micropollutant abatement. *Water Research*, **2024**, 254, 121388.
9. J. Chowdhury, C. Fricke, O. Bamidele, M. Bello, W. Yang, A. Heyden, G. Terejanu, Invariant Molecular Representations for Heterogeneous Catalysis. *J. Chem. Inf. Model.* **2024**, 64, 2, 327–339.

10. R. Zou[#], W. Yang[#], B. Rezaei, K. Tang, K. Guo, S. S. Keller, H. R. Andersen, and Y. Zhang, On the mechanism and selectivity of a novel iodine/peracetic acid process for the efficient and rapid elimination of micropollutants. *Chemical Engineering Journal* **2024**, 479, 147815. ***([#]Co-first author)***
11. Z. Sun, C. Zhi, Y. Sun, A. Bao, W. Yang, J. Yang, J. Hu, G. Liu, Rational construction of triple phase reaction zone using CuO-based heterostructure nanoarray for enhanced water oxidation reaction. *Inorganic Chemistry* **2023**, 62, 51, 21461–21469.
12. D. Zhang[#], W. Yang[#], Z. Wang, C. Ren, Y. Wang, M. Ding, T. Liu, Efficient electrochemical CO2 reduction reaction on a robust perovskite type cathode with in-situ exsolved Fe-Ru alloy nanocatalysts. *Separation and Purification Technology* **2023**, 304, 122287. ***([#]Co-first author)***
13. J. Gopeesingh, R. Zhu, R. Schuarca, W. Yang, A. Heyden, J. Q Bond, Kinetic and Mechanistic Analysis of the Hydrodeoxygenation of Propanoic Acid on Pt/SiO_2. *Industrial & Engineering Chemistry Research* **2021**, 60 (45), 16171-16187.
14. B. Rajbanshi, W. Yang, A. Yonge, S. K. Kundu, C. Fricke, A. Heyden, Computational Investigation of the Catalytic Hydrodeoxygenation of Propanoic Acid over a Cu (111) Surface. *The Journal of Physical Chemistry C* **2021**, 125 (35), 19276-19293.
15. A. J Chowdhury[#], W. Yang[#], A. Heyden, G. A Terejanu, Comparative Study on the Machine Learning-Based Prediction of Adsorption Energies for Ring and Chain Species on Metal Catalyst Surfaces, *The Journal of Physical Chemistry C* **2021**, 125 (32), 17742-17748. ***([#]Co-first author)***
16. S. K Kundu, R. Vijay Solomon, W. Yang, E. Walker, O. Mamun, J. Q Bond, A. Heyden, Surface structure sensitivity of hydrodeoxygenation of biomass-derived organic acids over palladium catalysts: a microkinetic modeling approach. *Catalysis Science & Technology* **2021**, 11 (18), 6163-6181.
17. W. Yang, R. V Solomon, O. Mamun, J. Q Bond, A. Heyden, Investigation of the reaction mechanism of the hydrodeoxygenation of propionic acid over a Rh (1 1 1) surface: A first principles study. *Journal of Catalysis* **2020**, 391, 98-110.
18. W. Yang, Z. Wang, W. Tan, R. Peng, X. Wu, Y. Lu, First principles study on methane reforming over Ni/TiO2 (110) surface in solid oxide fuel cells under dry and wet atmospheres. *Sci. China Mater*. **2020**, 63, 364–374.
19. W. Yang, R.V. Solomon, J. Lu, O. Mamun, J.Q. Bond, A. Heyden*, Unraveling the mechanism of the hydrodeoxygenation of propionic acid over a Pt (111) surface in vapor and liquid phases, *Journal of Catalysis **2020,*** 381, 547-560.
20. M. Zare, R. V Solomon, W. Yang, A. Yonge, A. Heyden, Theoretical investigation of solvent effects on the hydrodeoxygenation of propionic acid over a Ni (111) catalyst model, *The Journal of Physical Chemistry C* **2020**, 124 (30), 16488-16500.
21. A. J. Chowdhury, W. Yang, K. E. Abdelfatah, M. Zare, A. Heyden*, G. A. Terejanu*, A Multiple Filter Based Neural Network Approach to the Extrapolation of Adsorption Energies on Metal Surfaces for Catalysis Applications, *J. Chem. Theory Comput.* **2020**, 16, 2, 1105-1114.
22. K. Abdelfatah[#], W. Yang[#], R.V. Solomon, B. Rajbanshi, A. Chowdhury, M. Zare, S. Kundu, A. Yonge, A. Heyden*, G. Terejanu*, Prediction of transition state energies of hydrodeoxygenation reactions on transition metal surfaces based on machine learning.

J. Phys. Chem. C **2019**, 123, 29804-29810. ***(#Co-first author)***

23. A. J. Chowdhury, W. Yang, E. Walker, O. Mamun, A. Heyden, and G. A. Terejanu, Prediction of Adsorption Energies for Chemical Species on Metal Catalyst Surfaces Using Machine Learning. *J. Phys. Chem. C* **2018**, 122, 28142-28150.
24. W. Tan, D. Huan, W. Yang, N. Shi, W. Wang, R. Peng, X. Wu and Y. Lu, A first-principles study on divergent reactions of using a $Sr_3Fe_2O_7$ cathode in both oxygen ion conducting and proton conducting solid oxide fuel cells. *RSC Adv.,* **2018**, 8, 26448–26460.
25. Y. Xi, W. Yang, S. Cheettu Ammal, J. Lauterbach, Y. Pagan-Torres and A. Heyden, Mechanistic study of the ceria supported, recatalyzed deoxydehydration of vicinal OH groups. *Catal. Sci. Technol.* **2018**, 8, 5740-5752.
26. M. Li, Z. Sun, W. Yang, T. Hong, Z. Zhu, Y. Zhang, X. Wu and C. Xia, Mechanism for the enhanced oxygen reduction reaction of $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_3$ by strontium carbonate, *Phys. Chem. Chem. Phys.*, **2017**, 19, 503-509.
27. Z. Wang, W. Yang, L. Bi, Z. Wang, C. Xia, R. Peng, Y. Lu. A high-performance cathode for proton conducting solid oxide fuel cells, *J. Mater. Chem. A*, **2015**, 3, 8405-8412.
28. W. Yang, Z. Wang, C. Xia, R. Peng, X. Wu, Y. Lu, Enhanced catalytic activity toward O_2 reduction on Pt-modified $La_{1-x}Sr_xCo_{1-y}Fe_yO_{3-\delta}$cathode: A combination study of first-principles calculation and experiment. *ACS Appl. Mater. Interfaces*, **2014**, 6, 21051−21059.
29. Z. Wang, Z. Wang, W. Yang, R. Peng, Y. Lu. Carbon-tolerant solid oxide fuel cells using $NiTiO_3$ as an anode internal reforming layer. *Journal of Power Sources,* **2014**, 255, 404-409.
30. Z. Wang, W. Yang, C. Xia, R. Peng, X. Wu, Y. Lu. First-principles study of O_2 reduction on $BaZr_{1-x}Co_xO_3$ cathodes in protonic-solid oxide fuel cells. *J. Mater. Chem. A*, **2014**, 2, 16707-16714.

ACADEMIC ACTIVITIES

Academic Conference

- A combination of density functional theory and machine learning to address large reaction network*, 2019****, the 26th meeting of the North American Catalysis Society****, Chicago, IL.*
- A Combination of Density Functional Theory and Machine Learning to Address Large Reaction Network, *2018* ***AIChE Annual Meeting****, Pittsburgh, PA*.
- Theoretical investigation of the Pt catalyzed hydrodeoxygenation of succinic acid to 1,4-butanediol, *2018* ***International Conference on Theoretical Aspects of Catalysis****, Los Angeles, California*.
- Rational Design of Heterogeneous Catalysts for Hydrodeoxygenation (HDO) of Succinic Acid – Platinum Catalyzed Hydrodeoxygenation of Succinic Acid to 1,4-Butanediol, *2017* ***Southeastern Catalysis Society Meeting****, Asheville, North Carolina*.
- Enhanced catalytic activity toward O_2 reduction on Pt-modified $La_{1-x}Sr_xCo_{1-y}Fe_yO_{3-\delta}$ cathode: A combination study of first-principles calculation and experiment, 2014 ***International Conference on Theoretical and High-Performance Computational***

Chemistry (ICT-HPCC), Beijing, China.

Scientific Journal Peer Review

- *ACS Catalysis*, *ACS Sustainable Chemistry & Engineering*, *Applied Catalysis B: Environment and Energy*, *Science China Materials*, *Energies*, *Journal of Physical Chemistry C*, *Journal of Catalysis*, *Catalyst*, *Clean Technologies*, *Nanomaterials*, *Nature Communications*, *Materials*, *Theoretical Chemistry Accounts*

AWARDS

- Kokes Award, the 26th meeting of the North American Catalysis Society, *06/23/2019.*
- Silver Prize of Best Posters, International Conference on Theoretical and High-Performance Computational Chemistry (ICT-HPCC). *Sept. 18, 2014.*
- 3 times Third Grade Scholarship, University of Science and Technology of China, *09/10/2009-10/11/2010.*