

Chao Yang

✉ c_yang@nus.edu.sg | 🌐 Y-Chao

12 Science Drive 2, Singapore 117549

OBJECTIVE

Postdoctoral Researcher at the National University of Singapore with over four years of interdisciplinary research experience in experimental catalysis, atomistic simulations, and AI-driven catalyst discovery. Expertise in density functional theory (DFT), ab initio and machine learning molecular dynamics (AIMD/MLMD), machine learning interatomic potentials (MLIPs) for investigating catalytic reaction mechanisms and accelerating material design and interface stability for energy conversion.

EXPERIENCE & EDUCATION

2026	National University of Singapore [🌐] Research Fellow. Advisor: Asst. Prof. Pengfei Ou	Singapore, Singapore
2024	Fudan University Ph. D. in Inorganic Chemistry. Advisor: Prof. Gengfeng Zheng	Shanghai, China
2020	Fudan University M. Sc. in Inorganic Chemistry. Advisor: Prof. Gengfeng Zheng	Shanghai, China
2017	Wuhan University of Technology B. Sc. in Materials Science and Engineering. Advisor: Prof. Liqiang Mai	Wuhan, China

PROJECTS

Project A: MLIP accelerated materials exploration <i>Tools: Pytorch, ML,</i> - Force components-to-similarity: assessing MLIP accuracy in force Prediction - MLIP facilitated understanding of catalyst dissolution, reconstruction and growth process	2024-present
Project B: Solid oxide electrolytic cells design <i>Tools: DFT, Reactor design, catalysts design</i> Conductive cation traps for synthesizing efficient and stable perovskite catalysts	2023-2023
Project C: Applications of DFT and machine learning to catalytic reactions <i>Tools: Bayesian posterior sampling, DFT, constant-potential simulation</i> - The Bayesian posterior sampling for kinetic parameters analysis - The source of hydrogen determines CO/CO₂ electroreduction to ethanol by kinetics analysis - Understanding the CO reduction mechanism under constant potential	2022-2024
Project D: Cascade reaction and reactor design <i>Tools: 3D modeling, Finite element analysis</i> - CN coupling by coupled nitrate reduction in series reactors - Membrane electrode assembly reactor modeling and fabrication - Understanding the CO reduction mechanism under constant potential	2020-2024
Project E: Nanocatalysts design <i>Tools: Synthesis of inorganic nanomaterials, Nanomaterial characterization</i> - Study on metal single-atom and cluster catalysts for CO₂ reduction performance - Preparation of Grain Boundary Rich CopperBased Catalysts	2017-2020

SKILLS

- Programming Languages:** Python, Fortran
- Plot Technologies:** Matplotlib, Plotly, Blender, 3DMax

- **Database Systems:** Mongodb
- **Data Science & Machine Learning:** Scipy, Pytorch
- **HPC maintance:** Slurm, PBS, Environment Module
- **Research Skills:** Catalytic reaction mechanism, catalyst design, interface simulation

PUBLICATIONS

 Total citations: 5,412 | *h*-index: 34 | *i10*-index: 42 (July 2026)

J=Journal, P=Submitted, †=Co-author

- [J1] Tengfei Li†, Chao Yang†, Kaiyang Li, Anxiang Guan, Yali Ji, Ximeng Lv, Yueli Quan, Qihao Wang, Gengfeng Zheng*. “Surface Hydrogen Mediated Formate Formation in CO₂ Electroreduction”. In: **The Journal of Physical Chemistry C** (2026).
- [J2] Huijun Lv†, Chao Yang†, Minghao Sun, Yu Yang, Fengwang Li, Pengfei Ou*, Yuhang Wang*. “Bipolar membranes reveal surface-hydroxyl-structure-dependent water dissociation mechanism”. In: **Nature Communications** (2026).
- [P3] Chao Yang, Pengfei Ou. “Ru Oxidation State Governs Competing Oxygen Evolution and Dissolution Pathways on RuO₂ in Water”. In: **Submitted** (2026).
- [P4] Chao Yang, Gengfeng Zheng. “Kinetic parameters guiding adsorbed hydrogen engineering for ethanol formation in CO₂ reduction”. In: **Submitted** (2026).
- [J5] Chao Yang, Pengfei Ou. “Heterogeneous catalyst design by generative models”. In: **Journal of Materials Informatics** 5.4 (2025), N–A.
- [J6] Chao Yang, Yaqin Yan, Yuncheng Hu, Yangshen Chen, Anxiang Guan, Cejun Hu, Lijuan Zhang, Gengfeng Zheng*. “Promoting CO Electroreduction to C₂+ Oxygenates by Distribution of Water Dissociation Sites”. In: **Small Methods** 9.1 (2025), p. 2400393.
- [J7] Chengwei Yang†, Chao Yang†, Yunxia Liang, Hongxia Yan, Aodi Zhang, Guixian Ge, Wentao Wang, Pengfei Ou. “Machine-learning enables nitrogen reduction reaction on transition metal doped C₃B by controlling the charge states”. In: **Materials Chemistry Frontiers** 9.11 (2025), pp. 1681–1689.
- [J8] Chengwei Yang†, Chao Yang†, Hongxia Yan, Guixian Ge, Wentao Wang, Pengfei Ou. “Charge-state-regulated transition metal doped g-C₃N₃ for the electrochemical nitrogen reduction reaction: defect physics and constant potential study”. In: **Journal of Materials Chemistry A** 13.45 (2025), pp. 39032–39041.
- [J9] Quan Zhang†, Chao Yang†, Yangshen Chen, Yaqin Yan, Miao Kan, Huining Wang, Ximeng Lv, Qing Han, Gengfeng Zheng*. “Efficient Photocatalytic CH₄-to-Ethanol Conversion by Limiting Interfacial Hydroxyl Radicals Using Gold Nanoparticles”. In: **Angewandte Chemie** 137.7 (2025), e202419282.
- [J10] Qihao Wang†, Chao Yang†, Yaqin Yan, Haisheng Yu, Anxiang Guan, Miao Kan, Quan Zhang, Lijuan Zhang, Gengfeng Zheng*. “Electrocatalytic CO₂ Upgrading to Triethanolamine by Bromine-Assisted C₂H₄ Oxidation”. In: **Angewandte Chemie International Edition** 62.5 (2023), e202212733.
- [J11] Anxiang Guan†, Chao Yang†, Qihao Wang, Linping Qian, Jinyuan Cao, Lijuan Zhang, Limin Wu, Gengfeng Zheng*. “Atomic-level copper sites for selective CO₂ electroreduction to hydrocarbon”. In: **ACS sustainable chemistry & engineering** 9.40 (2021), pp. 13536–13544.
- [J12] Chao Yang, Yuhang Wang, Linping Qian, Abdullah M Al-Enizi, Lijuan Zhang, Gengfeng Zheng*. “Heterogeneous electrocatalysts for CO₂ reduction”. In: **ACS Applied Energy Materials** 4.2 (2021), pp. 1034–1044.
- [J13] Chao Yang, Hanchen Shen, Anxiang Guan, Junlang Liu, Tengfei Li, Yali Ji, Abdullah M Al-Enizi, Lijuan Zhang, Linping Qian, Gengfeng Zheng*. “Fast cooling induced grain-boundary-rich copper oxide for electrocatalytic carbon dioxide reduction to ethanol”. In: **Journal of colloid and interface science** 570 (2020), pp. 375–381.

- [J14] Anxiang Guan, Chao Yang, Yueli Quan, Hanchen Shen, Na Cao, Tengfei Li, Yali Ji, Gengfeng Zheng*. "One-dimensional Nanomaterial Electrocatalysts for CO₂ Fixation". In: **Chemistry—An Asian Journal** 14.22 (2019), pp. 3969–3980.
- [J15] Tengfei Li, Chao Yang, Jing-Li Luo, Gengfeng Zheng*. "Electrolyte driven highly selective CO₂ electroreduction at low overpotentials". In: **ACS Catalysis** 9.11 (2019), pp. 10440–10447.
- [J16] Lu Song, Chao Yang, Huining Wang, Yuanyuan Xue, Ximeng Lv, Cejun Hu, Lijuan Zhang, Gengfeng Zheng*. "Discovering Descriptors for CO₂-to-Methanol Electrosynthesis on Cu-Based Alloy Catalysts by Machine Learning". In: **Advanced Sustainable Systems** 9.12 (2025), e01190.
- [J17] Bowen Wu, Lu Song, Hairui Ma, Kewei Zhang, Mingtai Liu, Anxiang Guan, Zhengzheng Liu, Chao Yang, Naixin Lyu, Gengfeng Zheng. "Enhancing surface electron donation of single-atom copper catalyst for promoting CO₂ electroreduction to CH₄". In: **Chemical Engineering Journal** (2025), p. 170710.
- [J18] Yuanyuan Xue, Ximeng Lv, Chao Yang, Lu Song, Lijuan Zhang, Gengfeng Zheng*. "Promoting electrocatalytic CO₂ reduction to n-propanol over ethanol at Cu step sites". In: **Chemical Science** 16.30 (2025), pp. 13944–13950.
- [J19] Yaqin Yan, Chao Yang, Huining Wang, Cejun Hu, Pei Yuan, Lijuan Zhang, Gengfeng Zheng*. "Efficient Photocatalytic Ethylene Oxidation to Acetaldehyde by Asymmetrical Dehydrogenation". In: **Small** 21.30 (2025), p. 2503710.
- [J20] Fan Zhang, Ximeng Lv, Haozhen Wang, Junzhuo Cai, Huining Wang, Shuai Bi, Ruilin Wei, Chao Yang, Gengfeng Zheng*, Qing Han*. "p- π Conjugated Covalent Organic Frameworks Expedite Molecular Triplet Excitons for H₂O₂ Production Coupled with Biomass Upgrading". In: **Advanced Materials** 37.17 (2025), p. 2502220.
- [J21] Jing Zhang, Yan Liu, Chao Yang, Yanyan Qu, Aodi Zhang, Zhenzhen Feng, Wentao Wang, Pengfei Ou. "Design of bifunctional oxygen evolution/reduction electrocatalysts on g-C₃N₃ monolayer by a defect physics method". In: **Journal of Catalysis** 447 (2025), p. 116135.
- [J22] Yangshen Chen, Naixin Lyu, Junbo Zhang, Shuai Yan, Chen Peng, Chao Yang, Ximeng Lv, Cejun Hu, Min Kuang, Gengfeng Zheng*. "Tailoring the* CO and* H Coverage for Selective CO₂ Electroreduction to CH₄ or C₂H₄". In: **Small** 20.15 (2024), p. 2308004.
- [J23] Huiying Deng, Tingting Liu, Wenshan Zhao, Jundong Wang, Yuesheng Zhang, Shuzhen Zhang, Yu Yang, Chao Yang, Wenzhi Teng, Zhuo Chen. "Substituent tuning of Cu coordination polymers enables carbon-efficient CO₂ electroreduction to multi-carbon products". In: **Nature Communications** 15.1 (2024), p. 9706.
- [J24] Yali Ji, Ximeng Lv, Ruilin Wei, Anxiang Guan, Chao Yang, Yaqin Yan, Min Kuang, Gengfeng Zheng*. "Unconventional Electrocatalytic CO Conversion to C₂ Products on Single-Atomic Pd-Agn Sites". In: **Angewandte Chemie International Edition** 63.43 (2024), e202411194.
- [J25] Naixin Lyu, Yangshen Chen, Anxiang Guan, Ruilin Wei, Chao Yang, Yuhang Huang, Ximeng Lv, Cejun Hu, Min Kuang, Gengfeng Zheng*. "Electrocatalytic glycerol upgrading into glyceric acid on Ni₃Sn intermetallic compound". In: **Small** 20.35 (2024), p. 2401872.
- [J26] Xuan Wang, Ruihu Lu, Binbin Pan, Chao Yang, Mengjiao Zhuansun, Jun Li, Yi Xu, Sung-Fu Hung, Gengfeng Zheng, Yanguang Li*. "Enhanced carbon-carbon coupling at interfaces with abrupt coordination number changes". In: **ChemSusChem** 17.15 (2024), e202400150.
- [J27] Yaqin Yan, Kunhao Liu, Chao Yang, Yangshen Chen, Ximeng Lv, Cejun Hu, Lijuan Zhang, Gengfeng Zheng*. "Electrokinetic Analysis-Driven Promotion of Electrocatalytic CO Reduction to n-Propanol". In: **Small** 20.50 (2024), p. 2406345.
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- [J29] Chengfeng Zhao, Chao Yang, Ximeng Lv, Shengyao Wang, Cejun Hu, Gengfeng Zheng, Qing Han. "Bipolaronic motifs induced spatially separated catalytic sites for tunable syngas photosynthesis from CO₂". In: **Advanced Materials** 36.25 (2024), p. 2401004.

- [J30] Feini Hao, Chao Yang, Ximeng Lv, Fangshuai Chen, Shengyao Wang, Gengfeng Zheng*, Qing Han*. "Photo-driven quasi-topological transformation exposing highly active nitrogen cation sites for enhanced photocatalytic H₂O₂ production". In: **Angewandte Chemie International Edition** 62.50 (2023), e202315456.
- [J31] Shuyi Kong, Ximeng Lv, Xin Wang, Zhengzheng Liu, Zichuang Li, Bingquan Jia, Du Sun, Chao Yang, Lijia Liu, Anxiang Guan. "Delocalization state-induced selective bond breaking for efficient methanol electrosynthesis from CO₂". In: **Nature Catalysis** 6.1 (2023), pp. 6–15.
- [J32] Ximeng Lv, Zhengzheng Liu, Chao Yang, Yali Ji, Gengfeng Zheng*. "Tuning structures and microenvironments of Cu-based catalysts for sustainable CO₂ and CO electroreduction". In: **Accounts of Materials Research** 4.3 (2023), pp. 264–274.
- [J33] Anxiang Guan, Yalei Fan, Shibo Xi, Haoliang Huang, Quan Zhang, Naixin Lyu, Bowen Wu, Yangshen Chen, Zhengzheng Liu, Chao Yang. "Nitrogen-adsorbed hydrogen species promote CO₂ methanation on Cu single-atom electrocatalyst". In: **ACS Materials Letters** 5.1 (2022), pp. 19–26.
- [J34] Yali Ji, Zheng Chen, Ruilin Wei, Chao Yang, Yuhang Wang, Jie Xu, Hao Zhang, Anxiang Guan, Jiatang Chen, Tsun-Kong Sham. "Selective CO-to-acetate electroreduction via intermediate adsorption tuning on ordered Cu–Pd sites". In: **Nature Catalysis** 5.4 (2022), pp. 251–258.
- [J35] Miao Kan, Chao Yang, Qihao Wang, Quan Zhang, Yaqin Yan, Kunhao Liu, Anxiang Guan, Gengfeng Zheng*. "Defect-assisted electron tunneling for photoelectrochemical CO₂ reduction to ethanol at low overpotentials". In: **Advanced Energy Materials** 12.26 (2022), p. 2201134.
- [J36] Kunhao Liu, Chao Yang, Ruilin Wei, Xingyu Ma, Chen Peng, Zhengzheng Liu, Yangshen Chen, Yaqin Yan, Miao Kan, Yaoyue Yang. "Unraveling and tuning the linear correlation between CH₄ and C₂ production rates in CO₂ electroreduction". In: **Science Bulletin** 67.10 (2022), pp. 1042–1048.
- [J37] Zhengzheng Liu, Jinyuan Cao, Bowen Wu, Linping Qian, Anxiang Guan, Chao Yang, Ximeng Lv, Lijuan Zhang, Gengfeng Zheng*. "Surface energy tuning on Cu/NC catalysts for CO electroreduction". In: **ACS Catalysis** 12.20 (2022), pp. 12555–12562.
- [J38] Zhengzheng Liu, Ximeng Lv, Junbo Zhang, Anxiang Guan, Chao Yang, Shuai Yan, Yangshen Chen, Kunhao Liu, Gengfeng Zheng*. "Hydroxy-group-enriched In₂O₃ facilitates CO₂ electroreduction to formate at large current densities". In: **Advanced Materials Interfaces** 9.6 (2022), p. 2101956.
- [J39] Haozhen Wang, Chao Yang, Fangshuai Chen, Gengfeng Zheng*, Qing Han*. "A crystalline partially fluorinated triazine covalent organic framework for efficient photosynthesis of hydrogen peroxide". In: **Angewandte Chemie International Edition** 61.19 (2022), e202202328.
- [J40] Jing Wang, Yangshen Chen, Shishi Zhang, Chao Yang, Jun-Ye Zhang, Yaqiong Su, Gengfeng Zheng*, Xiaosheng Fang*. "Controllable States and Porosity of Cu-Carbon for CO₂ Electroreduction to Hydrocarbons". In: **Small** 18.37 (2022), p. 2202238.
- [J41] Chongbei Wu, Zhenyuan Teng, Chao Yang, Fangshuai Chen, Hong Bin Yang, Lei Wang, Hangxun Xu, Bin Liu, Gengfeng Zheng*, Qing Han*. "Polarization engineering of covalent triazine frameworks for highly efficient photosynthesis of hydrogen peroxide from molecular oxygen and water". In: **Advanced Materials** 34.28 (2022), p. 2110266.
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- [J44] Anxiang Guan, Qihao Wang, Yali Ji, Si Li, Chao Yang, Linping Qian, Lijuan Zhang, Limin Wu, Gengfeng Zheng*. "Steric effect induces CO electroreduction to CH₄ on Cu–Au alloys". In: **Journal of Materials Chemistry A** 9.38 (2021), pp. 21779–21784.

- [J45] Yali Ji, Chao Yang, Linping Qian, Lijuan Zhang, Gengfeng Zheng*. “Promoting electrocatalytic carbon monoxide reduction to ethylene on copper-polypyrrole interface”. In: **Journal of Colloid and Interface Science** 600 (2021), pp. 847–853.
- [J46] Si Li, Anxiang Guan, Chao Yang, Chen Peng, Ximeng Lv, Yali Ji, Yueli Quan, Qihao Wang, Lijuan Zhang, Gengfeng Zheng*. “Dual-atomic Cu sites for electrocatalytic CO reduction to C₂+ products”. In: **ACS Materials Letters** 3.12 (2021), pp. 1729–1737.
- [J47] Yueli Quan, Ruohan Yu, Jiexin Zhu, Anxiang Guan, Ximeng Lv, Chao Yang, Si Li, Jinsong Wu, Gengfeng Zheng*. “Efficient carboxylation of styrene and carbon dioxide by single-atomic copper electrocatalyst”. In: **Journal of colloid and interface science** 601 (2021), pp. 378–384.
- [J48] Qihao Wang, Tengfei Li, Chao Yang, Menghuan Chen, Anxiang Guan, Li Yang, Si Li, Ximeng Lv, Yuhang Wang, Gengfeng Zheng*. “Electrocatalytic methane oxidation greatly promoted by chlorine intermediates”. In: **Angewandte Chemie** 133.32 (2021), pp. 17538–17543.
- [J49] Shuai Yan, Chen Peng, Chao Yang, Yangshen Chen, Junbo Zhang, Anxiang Guan, Ximeng Lv, Haozhen Wang, Zhiqiang Wang, Tsun-Kong Sham. “Electron localization and lattice strain induced by surface lithium doping enable ampere-level electrosynthesis of formate from CO₂”. In: **Angewandte Chemie** 133.49 (2021), pp. 25945–25949.
- [J50] Na Cao, Yueli Quan, Anxiang Guan, Chao Yang, Yali Ji, Lijuan Zhang, Gengfeng Zheng*. “Oxygen vacancies enhanced cooperative electrocatalytic reduction of carbon dioxide and nitrite ions to urea”. In: **Journal of colloid and interface science** 577 (2020), pp. 109–114.
- [J51] Anxiang Guan, Zheng Chen, Yueli Quan, Chen Peng, Zhiqiang Wang, Tsun-Kong Sham, Chao Yang, Yali Ji, Linping Qian, Xin Xu. “Boosting CO₂ electroreduction to CH₄ via tuning neighboring single-copper sites”. In: **ACS energy letters** 5.4 (2020), pp. 1044–1053.
- [J52] Yulu Yang, Yang Tang, Haomin Jiang, Yongmei Chen, Pingyu Wan, Maohong Fan, Rongrong Zhang, Sana Ullah, Lun Pan, Ji-Jun Zou. “2020 Roadmap on gas-involved photo-and electrocatalysis”. In: **Chinese Chemical Letters** 30.12 (2019), pp. 2089–2109.
- [J53] Di Yuan, Zengxi Wei, Peng Han, Chao Yang, Linsong Huang, Zhengxiang Gu, Yu Ding, Jianmin Ma, Gengfeng Zheng*. “Electron distribution tuning of fluorine-doped carbon for ammonia electrosynthesis”. In: **Journal of Materials Chemistry A** 7.28 (2019), pp. 16979–16983.
- [J54] Yiliguma Yiliguma, Zhijie Wang, Chao Yang, Anxiang Guan, Longmei Shang, Abdullah M Al-Enizi, Lijuan Zhang, Gengfeng Zheng*. “Sub-5 nm SnO₂ chemically coupled hollow carbon spheres for efficient electrocatalytic CO₂ reduction”. In: **Journal of Materials Chemistry A** 6.41 (2018), pp. 20121–20127.
- [J55] Kwadwo Asare Owusu, Longbing Qu, Jiantao Li, Zhaoyang Wang, Kangning Zhao, Chao Yang, Kalele Mulonda Hercule, Chao Lin, Changwei Shi, Qiulong Wei. “Low-crystalline iron oxide hydroxide nanoparticle anode for high-performance supercapacitors”. In: **Nature communications** 8.1 (2017), p. 14264.

HONORS AND AWARDS

The 3rd Hackathon Competition *Electrochemical*

2023-Second prize

Deepmodeling community

- Design the automated workflow for reduction potential prediction
- Understanding the machine learning interatomic potential accelerates simulation

Internet+ Innovation and Entrepreneurship Competition, Shanghai Division

2021-Second prize

Shanghai Municipal Education Commission

- Advance CO₂ electroreduction toward practical application through membrane-integrated electrode design
- Identify key factors via techno-economic analysis and multi-physics field simulations

Postgraduate Outstanding Academic Scholarship

2017-Level 1

Fudan University

Outstanding Graduate

2015-School level

Wuhan University of Technology

ADDITIONAL INFORMATION

Languages: English, Chinese

Interests: Badminton, Swim, Basketball