Chao YANG

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Personal Profile

A postdoctoral researcher from the National University of Singapore is enrolled in machine-learning-assisted catalyst research. Dedicated to the conversion of CO_2 into high value-added chemicals, having four or more years of expertise, and specializing in **Machien learning techniques, DFT calculation, and catalyst design**. The search was mainly for the field of theory simulation on $CO_{(2)}$ electro-reaction, the competition of selectivity, and kinetic study and exploration of intrinsic activity of catalysis.

Education

Fudan University — *Shanghai*
Ph. D. in Inorganic Chemistry, Nano New Energy Materials — *Sept 2020 - June 2024*

Fudan University — *Shanghai*
M. Sc. in Inorganic Chemistry, Nano New Energy Materials — *Sep 2017 - June 2020*

Wuhan University of Technology — *Wuhan, Hubei*
B. Sc. in Materials Science and Engineering — *Apr 2013 - Apr 2017*

Achievements

2023	**Second Prize**, The 3rd Hackathon Competition Electrochemical Track of Deepmodeling Community	*Xiamen*
2021	**Second Prize**, Internet+ Innovation and Entrepreneurship Competition, Shanghai Division	*Shanghai*
2020	**Second Prize**, Fanhai Cup Innovation and Entrepreneurship, Fudan University	*Shanghai*
2019	**318/340**, Graduate Record Examinations (GRE)	*Shanghai*
2017	**Level 1**, Postgraduate Outstanding Academic Scholarship	*Shanghai*
2017	**School level**, Outstanding Graduate of Wuhan University of Technology	*Wuhan*
2015	**Level 1**, Wuhan University of Technology Scholarship	*Wuhan*
2015	**532/710**, College English Test Band 6	*Wuhan*

Work & Research Experience

National University of Singapore — *Singapore, Singapore*
AI-enhanced catalyst simulation, advisor: Pengfei Ou — *Oct 2024 - Oct 2025*

- Machine learning potential facilitated understanding of catalyst dissolution process
- Surface reconstruction promoted CO_2 to $HCOO^-$ selectivity under sulfur oxide atmosphere

Soochow University — *Soochow, Jiangsu*
Solid oxide electrolytic cells design, advisor:Yuhang Wang — *May 2023 - Sep 2023*

- SOEC for CO_2 reduction and CH_4 oxidation reactions

Fudan University — *Shanghai*
Applications of DFT and machine learning to catalytic reactions — *Sep 2022 - Jun 2024*

- Weak CO adsorption sites for $CO_{(2)}$ electroreduction to ethanol by kinetics analysis
- DFT theoretical calculations of efficient electrochemical CO_2 reduction catalysts
- Reconstruction of alloy catalysts in CO atmosphere
- **Technical Skills:** DFT, Machine learning, Electrochemical fundamental

Fudan University — *Shanghai*
Casecade reaction and reactor design, supervisor: Gengfeng Zheng — *Sep 2020 - June 2024*

- C-N coupling by coupled nitrate reduction in series reactors
- Membranes electrode assembly reactor modeling and fabrication
- **Technical Skills:** 3D modeling, Finite element analysis

Fudan University — *Shanghai*
Nano-catalysts design, supervisor: Gengfeng Zheng — *Sep 2017 - Jun 2020*

- Study on metal single atom and cluster catalysts for CO_2 reduction performance
- Preparation of Grain Boundary Rich Copper-Based Catalysts

- **Technical Skills:** Synthesis of inorganic nanomaterials, Nanomaterial characterization

Wuhan University of Technology *Wuhan, Hubei*

Energy Storage Applications of Nanomaterials, supervisor: Liqiang Mai *Sep 2014 - Jun 2017*

- Amorphous iron oxide cathode for supercapacitor energy storage
- Synthesis and energy storage of lithium iron molybdate nanowires

Publications

†= CO-FIRST AUTHOR

1. Kinetic analysis linking proton effects to ethanol selectivity in electrochemical $CO_{(2)}$ reduction

Chao Yang, Gengfeng Zheng*

In preparation

2. Efficient Photocatalytic CH4-to-Ethanol Conversion by Limiting Interfacial Hydroxyl Radicals Using Gold Nanoparticles

Quan Zhang†, **Chao Yang**†, Yangshen Chen, Yaqin Yan, Miao Kan, Huining Wang, Ximeng Lv, Qing Han, Gengfeng Zheng*

Angew. Chem. Int. Ed., 2025, 2, e202419282

3. Promoting CO Electroreduction to C_{2+} Oxygenates by Distribution of Water Dissociation Sites

Chao Yang, Yaqin Yan, Yuncheng Hu, Yangshen Chen, Anxiang Guan, Lijuan Zhang*, Gengfeng Zheng*

Small Methods, 2024, doi: 10.1002/smtd.202400393.

4. Electrocatalytic CO_2 upgrading to triethanolamine by bromine-assisted C_2H_4 oxidation

Qihao Wang†, **Chao Yang**†, Yaqin Yan, Haisheng Yu, Anxiang Guan, Miao Kan, Quan Zhang, Linjuan Zhang, Gengfeng Zheng*

Angew. Chem. Int. Ed., 2023, 62, e202212733

5. Atomic-level copper sites for selective CO_2 electroreduction to hydrocarbon

Anxiang Guan†, **Chao Yang**†, Qihao Wang, Linping Qian*, Jinyuan Cao, Lijuan Zhang, Limin Wu, Gengfeng Zheng*

ACS Sustainable Chem. Eng., 2021, 9, 13536-13544

6. Heterogeneous Electrocatalysts for CO_2 Reduction

Chao Yang, Yuhang Wang, Linping Qian, Abdullah M. Al-Enizi, Lijuan Zhang*, Gengfeng Zheng*

ACS Appl. Energy Mater., 2021, 4, 1034-1044

7. Fast cooling induced grain-boundary-rich copper oxide for electrocatalytic carbon dioxide reduction to ethanol

Chao Yang, Hanchen Shen, Anxiang Guan, Junlang Liu, Tengfei Li, Yali Ji, Abdullah M. Al-Enizi, Lijuang Zhang, Linping Qian, Gengfeng Zheng*

J. Colloid Interf. Sci., 2020, 570, 375-381

8. A crystalline partially fluorinated triazine covalent organic framework for efficient photosynthesis of hydrogen peroxide

Haozhen Wang, **Chao Yang**, Fangshuai Chen, Gengfeng Zheng, Qing Han*

Angew. Chem. Int. Ed., 2022, 134, e202202328

9. Unraveling and tuning the linear correlation between CH_4 and C2 production rates in CO_2 electroreduction

Kunhao Liu, **Chao Yang**, Ruilin Wei, Xingyu Ma, Chen Peng, Zhengzheng Liu, Yangshen Chen, Yaqin Yan, Miao Kan, Yaoyue Yang, Gengfeng Zheng*

Sci. Bulletin, 2022, 67, 1042-1048

10. Electrolyte driven highly selective CO_2 electroreduction at low overpotentials

Tengfei Li, **Chao Yang**, Jing-Li Luo*, Gengfeng Zheng*

ACS Catal., 2019, 9, 10440-10447