



Chen Chen Er

Date of birth: 16/12/1997 | **Nationality:** Malaysian | **Phone number:** (+49) 1701051758 (Work) |

Email address: tidustide245@gmail.com | **Website:** <https://erchenchen.faculty.bio/> | **LinkedIn:** <https://www.linkedin.com/in/er-chen-chen-15a38816a/> |

Address: 387, JALAN SS 2/2, 47300, PETALING JAYA, Malaysia (Home) |

Address: August-Bebel-Straße 15B, 01219, Dresden, Germany (Work)

ABOUT ME

Computational Chemist specializing in Power-to-X technologies. Dr. Chen Chen Er's main research interest is on leveraging machine learning from first principles approach towards materials exploration and design. Having completed his doctoral studies in Chemical Engineering at Monash University in July 2023 and worked as a postdoctoral research fellow in Singapore and currently based in Germany, Dr. Er is equipped with a solid foundation in applying quantum chemistry modelling (i.e., VASP and LAMMPS) in a machine learning framework (self-coded using PyTorch and scikit-learn) to gain insights toward the rational development of materials for real-world applications.

WORK EXPERIENCE

TECHNISCHE UNIVERSITÄT DRESDEN – DRESDEN, GERMANY

Business or Sector Education | **Department** Professur für Theoretische Chemie | **Email** chen_chen.er@tu-dresden.de |

Website <http://theory.chm.tu-dresden.de/members.shtml?name=ccer>

RESEARCH FELLOW – 01/11/2024 – CURRENT

- Design and exploration of high-entropy ceramics for extreme engineering.

SINGAPORE UNIVERSITY OF TECHNOLOGY AND DESIGN – SINGAPORE, SINGAPORE

Business or Sector Professional, scientific and technical activities |

Department Science, Mathematics, and Technology Clusters | **Email** chenchen_er@sutd.edu.sg |

Website <https://www.sutd.edu.sg/>

RESEARCH FELLOW – 31/08/2023 – 31/05/2024

- Unravel the Origin and Mechanisms of Efficient Persistent Photocatalyst towards Resolving Solar Intermittency a priori.
- Quantum Modelling of Carrier Tunnelling Injection in 2D Semiconductor Device Contact Heterostructures.

SINGAPORE UNIVERSITY OF TECHNOLOGY AND DESIGN – SINGAPORE, SINGAPORE

Business or Sector Professional, scientific and technical activities |

Department Science, Mathematics, and Technology Clusters | **Email** chenchen_er@sutd.edu.sg |

Website <https://www.sutd.edu.sg/>

VISITING RESEARCH FELLOW – 22/04/2023 – 30/08/2023

- Unravel the Origin and Mechanisms of Efficient Persistent Photocatalyst towards Resolving Solar Intermittency a priori.
- Quantum Modelling of Carrier Tunnelling Injection in 2D Semiconductor Device Contact Heterostructures.

MONASH UNIVERSITY – SUBANG JAYA, MALAYSIA

Business or Sector Education | **Department** Department of Chemical Engineering | **Email** Chen.Er@monash.edu |

Website <https://www.monash.edu/>

PHD. STUDENT – 02/03/2020 – 26/07/2023

- Providing critical insights through fundamental guidance and theoretical evaluations of rational semiconductor design for CO₂ reduction applications through photocatalysis using density functional theory (DFT).
- Co-supervised undergraduate research projects in photocatalytic applications.
- Contributed to the setup of Vienna ab initio software simulation package (VASP) and related post-processing software in Monash High Performance Computing (HPC) infrastructure.

EDUCATION AND TRAINING

02/03/2020 – 26/07/2023 Subang Jaya, Malaysia

PHD. Monash University

- Providing critical insights through fundamental guidance and theoretical evaluations of rational semiconductor design for CO₂ reduction applications through photocatalysis using density functional theory (DFT).
- Co-supervised undergraduate research projects in photocatalytic applications.
- Contributed to the setup of Vienna ab initio software simulation package (VASP) and related post-processing software in Monash High Performance Computing (HPC) infrastructure.

Website <https://www.monash.edu/> | **Level in EQF** EQF level 8 | **National classification** Level 10 | **Type of credits** N/A. |

Number of credits N/A. |

Thesis Mechanistic Insights into the Fundamentals of Photocatalytic Reduction of Carbon Dioxide from First Principles Density Functional Theory Studies

Link [https://bridges.monash.edu/articles/thesis/](https://bridges.monash.edu/articles/thesis/Mechanistic_Insights_into_the_Fundamentals_of_Photocatalytic_Reduction_of_Carbon_Dioxide_from_First_Principles_Density_Functional_Theory_Studies/23690385)

[Mechanistic Insights into the Fundamentals of Photocatalytic Reduction of Carbon Dioxide from First Principles Density Functional Theory Studies](https://bridges.monash.edu/articles/thesis/Mechanistic_Insights_into_the_Fundamentals_of_Photocatalytic_Reduction_of_Carbon_Dioxide_from_First_Principles_Density_Functional_Theory_Studies/23690385)

02/02/2016 – 19/12/2019 Subang Jaya, Malaysia

BACHELOR IN CHEMICAL ENGINEERING (HONS.) Monash University

Website <https://www.monash.edu/> | **Field of study** Chemical engineering and processes | **Final grade** H2A |

Level in EQF EQF level 6 | **National classification** Level 9 | **Type of credits** ECTS | **Number of credits** 240

LANGUAGE SKILLS

Mother tongue(s): **CHINESE**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	C1	C1	C1	C1	C1
MALAY	B2	B2	B2	B2	B2

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

SKILLS

Presentation

Microsoft Office

Software

Materials Simulation: LAMMPS, NAMD, VASP | QUANTUM ESPRESSO | Matlab/Simulink

Technical Skills

Molecular modelling with Density-functional theory (DFT) | Reaction Mechanism Study Through Transition State Calculation

Knowledge

Heterogeneous Catalysis | HPC: SLURM, PBS | Operating Systems: UNIX, Linux, Solaris, VxWorks, Windows | IBM | Python library used for Scientific computing and technical computing(SciPy) | Python, Scikit-Learn, Numpy, Matplotlib | PyTorch, Keras

Hobby

Enjoy mountain hiking | Playing the piano (ABRSM Grade 5 Certification) | Sports running walking swimming climbing | Good in badminton

PUBLICATIONS

2025

[Interpretable Machine Learning Framework: Predicting Catalytic Activities of Complex Photocatalysts towards CO₂ Conversion](#)

Chen-Chen Er, Lutfi K Putri, Yee Sin Ang, Hui Ying Yang, Siang-Piao Chai (2025). Interpretable machine learning framework: Predicting catalytic activities of complex photocatalysts towards CO₂ conversion. Materials Today Physics, 57, 101800. (ISI top 10, JIF: 9.7)

2025

[Unveiling fundamental first-principles insights into single-atom transition metal photocatalysts for carbon dioxide reduction](#)

Chen-Chen Er, Lutfi K Putri, Yee Sin Ang, Siang-Piao Chai (2025). Unveiling fundamental first-principles insights into single-atom transition metal photocatalysts for carbon dioxide reduction. Fuel, 382, 133746. (JIF: 6.7)

2024

[The Big Problem in Surface Catalysis Modelling](#)

Chen-Chen Er, Yee Wen Teh, Xin Ying Kong, Sounghmin Bae, Yu Kumagai, Siang-Piao Chai, Yee Sin Ang (2024). The Big Problem in Surface Catalysis Modelling. ChemRxiv doi:10.26434/chemrxiv-2024-9mbrm.

2024

[Revised Fowler–Dubridge model for multiphoton over-barrier electron emission from two-dimensional materials](#)

Yi Luo, **Chen-Chen Er**, Yee Sin Ang, LK Ang. Revised Fowler–Dubridge model for multiphoton over-barrier electron emission from two-dimensional materials. Applied Physics Letters, 124, 10 (Q2, JIF: 4.0)

2024

[Computational Design of 2D Phosphorus Nanostructures for Renewable Energy Applications: A Review](#)

Chen-Chen Er, Cheng-May Fung, Wei-Kean Chong, Yong Jieh Lee, Lling-Lling Tan, Yee Sin Ang, Nikhil V Medhekar, Siang-Piao Chai (2024). Computational Design of 2D Phosphorus Nanostructures for Renewable Energy Applications: A Review. Advanced Electronic Materials, 10(7), 2300869. (JIF: 5.3)

2024

[MXene quantum dot-sensitized heterostructures for broad solar spectrum CO₂ reduction](#)

Cheng-May Fung, Boon-Junn Ng, Yi-Hao Chew, **Chen-Chen Er**, Jingxiang Low, Xuecheng Guo, Xin Ying Kong, Lling-Lling Tan, Hiroshi Onishi, Abdul Rahman Mohamed, Siang-Piao Chai (2024). MXene quantum dot-sensitized heterostructures for broad solar spectrum CO₂ reduction. Cell Reports Physical Science, 5(11), 102296. (JIF: 7.9)

2023

[Effective Low-Powered Photocatalytic Disinfection via Synchronous Introduction of Oxygen Dopants and Carbon Defects in Carbon Nitride](#)

Nur Atika Nikma Dahlan, Lutfi Kurnianditia Putri, **Chen-Chen Er**, Boon-Junn Ng, Chien Wei Ooi, Lling-Lling Tan, Siang-Piao Chai (2023). Effective Low-Powered Photocatalytic Disinfection via Synchronous Introduction of Oxygen Dopants and Carbon Defects in Carbon Nitride. ACS Applied Materials & Interfaces, 15, 46, 53371-53381. (Q1, JIF: 9.5)

2023

Engineering Nanoscale Homo-Heterojunction for Robust Z-Scheme CO₂ Conversion through Synchronous Amalgamation of Oxygen- Defective Ultrathin BiVO₄ and Red/Black Phosphorus

Cheng-May Fung, Boon-Junn Ng, **Chen-Chen Er**, Wei-Kean Chong, Jingxiang Low, Xuecheng Guo, Xin Ying Kong, Hing Wah Lee, Lling-Lling Tan, Abdul Rahman Mohamed, Siang-Piao Chai (2023). Engineering Nanoscale Homo-Heterojunction for Robust Z-Scheme CO₂ Conversion through Synchronous Amalgamation of Oxygen-Defective Ultrathin BiVO₄ and Red/Black Phosphorus. Small Structures, 4, 11, 2300083. (ISI top 10, JIF: 15.9)

2023

Toward Sustainable Ultrawide Bandgap van der Waals Materials: An ab initio Screening Effort

Chuin Wei Tan, Linqiang Xu, **Chen-Chen Er**, Siang-Piao Chai, Boris Kozinsky, Hui Ying Yang, Shengyuan A. Yang, Jing Lu, Yee Sin Ang (2023). Toward Sustainable Ultrawide Bandgap van der Waals Materials: An ab initio Screening Effort. Advanced Functional Materials. (ISI top 10, JIF: 19.0)

2023

Two-dimensional interface engineering of g-C₃N₄/g-C₃N₄ nanohybrid: Synergy between isotype and pn heterojunctions for highly efficient photocatalytic CO₂ reduction

Jie-Yinn Tang, **Chen-Chen Er**, Xin Ying Kong, Boon-Junn Ng, Yi-Hao Chew, Lling-Lling Tan, Abdul Rahman Mohamed, Siang-Piao Chai (2023). Two-dimensional interface engineering of g-C₃N₄/g-C₃N₄ nanohybrid: Synergy between isotype and pn heterojunctions for highly efficient photocatalytic CO₂ reduction. Chemical Engineering Journal, 466, 143287. (ISI top 10, JIF: 15.1)

2023

Sensitization of Bismuth Tungstate with Magnesium Phthalocyanine for Photoinduced Charge Redistribution and Electron Localization: CO₂ Photoreduction from Vis to NIR Region

Yee Wen Teh, Wei Kean Chong, **Chen-Chen Er**, Xin Ying Kong, Boon-Junn Ng, Siek Ting Yong, Siang-Piao Chai (2023). Sensitization of Bismuth Tungstate with Magnesium Phthalocyanine for Photoinduced Charge Redistribution and Electron Localization: CO₂ Photoreduction from Vis to NIR Region. Journal of Materials Chemistry C, 11, 705711. (Q1, JIF: 6.4)

2022

Insights from density functional theory calculations on heteroatom P-doped ZnIn₂S₄ bilayer nanosheets with atomic-level charge steering for photocatalytic water splitting

Wei-Kean Chong, Boon-Junn Ng, **Chen-Chen Er**, Lling-Lling Tan, Siang-Piao Chai (2022). Insights from density functional theory calculations on heteroatom P-doped ZnIn₂S₄ bilayer nanosheets with atomic-level charge steering for photocatalytic water splitting. Scientific Reports, 12, 1927. (Q2, JIF: 4.6)

2022

Unraveling the roles of single transition metal atom anchored on equivalent stoichiometry graphitic carbon nitride (gC₆N₆) for carbon dioxide reduction: a density functional theory study

Chen-Chen Er, Lutfi K. Putri, Nikhil V. Medhekar, Siang-Piao Chai (2022). Unraveling the roles of single transition metal atom anchored on equivalent stoichiometry graphitic carbon nitride (gC₆N₆) for carbon dioxide reduction: a density functional theory study. Journal of Physics D: Applied Physics, 56(2), 024004. (Q2, JIF: 3.4)

2022

Synergistic Hybridization of Twin-Induced Red/Black Phosphorus and Tungsten Oxide as Homo-Hetero Dynamic Dual Junctions for Z-Scheme CO₂ Photoreduction

Cheng-May Fung, Boon-Junn Ng, **Chen-Chen Er**, Xin Ying Kong, Lling-Lling Tan, Abdul Rahman Mohamed, Siang-Piao Chai (2022). Synergistic Hybridization of Twin-Induced Red/Black Phosphorus and Tungsten Oxide as Homo-Hetero

2022

[Allotropes selection apropos of photocatalytic CO₂ reduction from first principles studies](#)

Chen-Chen Er, Lutfi K. Putri, Boon-Junn Ng, Nikhil V. Medhekar, Siang-Piao Chai (2022). Allotropes selection apropos of photocatalytic CO₂ reduction from first principles studies. Materials Today Physics, 26, 100751. (ISI top 10, JIF: 11.5)

2022

[Charge Modulation at Atomic-Level through Substitutional Sulfur Doping into Atomically Thin Bi₂WO₆ toward Promoting Photocatalytic CO₂ Reduction](#)

Yee Wen Teh, **Chen-Chen Er**, Boon-Junn Ng, Xin Ying Kong, Siek-Ting Yong, Siang-Piao Chai (2022). Charge Modulation at Atomic-Level through Substitutional Sulfur Doping into Atomically Thin Bi₂WO₆ toward Promoting Photocatalytic CO₂ Reduction. ChemSusChem 15(14) e202200471. (Q1, JIF: 8.4)

2022

[Uncovering the multifaceted roles of nitrogen defects in graphitic carbon nitride for selective photocatalytic carbon dioxide reduction: a density functional theory study](#)

Jie-Yinn Tang*, **Chen-Chen Er***, Lling-Lling Tan, Yi-Hao Chew, Abdul Rahman Mohamed, and Siang-Piao Chai (2022). Uncovering the multifaceted roles of nitrogen defects in graphitic carbon nitride for selective photocatalytic carbon dioxide reduction: a density functional theory study. (*Both authors contributed equally) Physical Chemistry Chemical Physics, 24 (18), 11124-11130. (Q1, JIF: 3.3)

2021

[Red Phosphorus: An Up-and-Coming Photocatalyst on the Horizon for Sustainable Energy Development and Environmental Remediation](#)

Cheng-May Fung, **Chen-Chen Er**, Lling-Lling Tan, Abdul Rahman Mohamed, Siang-Piao Chai (2022). Red Phosphorus: An Up-and-Coming Photocatalyst on the Horizon for Sustainable Energy Development and Environmental Remediation. Chemical Reviews. 122, 3, 3879-3965. (ISI top 10, JIF: 62.1)

2021

[Atomistic Insights into the Reformation of CH₄ with CO₂ on Metal-Free gC₃N₄: Unraveling the Reaction Mechanisms Using First-Principles DFT Calculations](#)

Chen-Chen Er, Jie-Yinn Tan, Nikhil V. Medhekar, Siang-Piao Chai (2021). Atomistic Insights into the Reformation of CH₄ with CO₂ on Metal-Free gC₃N₄: Unraveling the Reaction Mechanisms Using First-Principles DFT Calculations. Journal of Physical Chemistry C, 125(42), 23021-23028. (Q2, JIF: 3.7)

2021

[Proton-functionalized graphitic carbon nitride for efficient metal-free disinfection of Escherichia Coli under low-power light irradiation](#)

Boon-Junn Ng, Muhammad Khosyi Musyaffa, **Chen-Chen Er**, Kulandai Arockia Rajesh Packiam, WP Cathie Lee, Lling-Lling Tan, Hing Wah Lee, Chien Wei Ooi, Siang-Piao Chai (2021). Proton-functionalized graphitic carbon nitride for efficient metal-free disinfection of Escherichia Coli under low-power light irradiation. Chemistry-A European Journal, 27(9), 3085-3090. (Q2, JIF: 4.3)

2020

[Insights on the Impact of Doping Levels in Oxygen-doped gCN and its Effects on Photocatalytic Activity](#)

Lutfi K. Putri, Boon-Junn Ng, **Chen-Chen Er**, Wee-Jun Ong, Wei Sea Chang, Abdul Rahman Mohamed, Siang-Piao Chai (2020). Insights on the Impact of Doping Levels in Oxygen-doped gCN and its Effects on Photocatalytic Activity. Applied Surface Science, 504, 144427. (ISI top 10, JIF: 6.7)

2020

Tuning the Electronic Band Structure of Graphitic Carbon Nitride by Breaking Intramolecular Bonds: A Simple and Effective Approach for Enhanced Photocatalytic Hydrogen Production

Michell KT Chee, **Chen-Chen Er**, Jie-Yinn Tang, Lling-Lling Tan, Wei Sea Chang, Siang-Piao Chai (2020). Tuning the Electronic Band Structure of Graphitic Carbon Nitride by Breaking Intramolecular Bonds: A Simple and Effective Approach for Enhanced Photocatalytic Hydrogen Production. Applied Surface Science, 529, 146600. (ISI top 10, JIF: 6.7)

NETWORKS AND MEMBERSHIPS

01/05/2020 – CURRENT Malaysia

Boards of Engineers Malaysia (BEM)

Graduate Engineer
Membership No.: G1182180A

01/02/2020 – CURRENT United Kingdoms

Institution of Chemical Engineers (IChemE)

Associate Member
Membership No.: 100216623

CONFERENCES AND SEMINARS

16/03/2025 – 21/03/2025 Regensburg, Germany.

Deutsche Physikalische Gesellschaft (DPG)-Frühjahrstagungen 2025

Poster Contribution: Modelling and Descriptor-based Synthesizability Analysis of High-Entropy Materials.

Link <https://regensburg25.dpg-tagungen.de/programm/assets/r25book.pdf>

2023 – 2023 Singapore

1st- International Conference on Low-Energy Digital Devices and Computing (ICLED-2023)

2023 – 2023 Singapore

Institute of Physics Singapore (IPS) 2023

2022 – 2022 Malaysia

Chulalongkorn University Thailand – Monash University Malaysia Bilateral Research Seminar on Catalysis 2022

HONOURS AND AWARDS

02/03/2020

Graduate Research Tuition Fee Waiver Scholarship – Monash University

100% tuition fee waiver up to the duration stated below:

- Doctoral degree - Three years, six months full-time equivalent from the date of course commencement until the scholarship end date or upon thesis submission; whichever is earlier.

Co-investigator, SUTD Kickstarter initiative (Award No: SKI 2021_04_01) – Singapore University of Technology and Design

SGD \$100,000

Topic: “Designing Nanostructure with Enhanced Charge Storing Capacity for Round-the-Clock Photocatalytic Energy Conversion”

National Supercomputing Centre (NSCC) 2nd Call for Projects Jan’24 Cycle – NSCC Singapore

(Project ID:15003684) **3,750,000 CPU hours**

Topic: “High-throughput screening of 2D nanomaterials for persistent photocatalysis.”

● TEACHING TRACK

01/02/2024 – 31/12/2024

Science for a Sustainable World [SUTD]

Adjunct Teaching Fellow

-This course focuses on the importance of sustainable development by creating awareness of climate change and the human impact on the environment. Based on the Sustainable Development Goals (SDGs) from the United Nations, this course will address issues and challenges related to sustainability in four main areas: green materials, clean water, sustainable energy, and biodiversity. Emphasis is placed on the knowledge of science and engineering approaches towards achieving sustainable development. This course aims to enhance students' critical thinking skills in analyzing strategies based on scientific facts and current technologies.

01/12/2023 – 31/12/2023

Compact Physical World for SUTD-Polytechnic Special Arrangement [SUTD]

Ad hoc Teaching Fellow

-Emphasis on providing students with the ability to understand and explain the inner mechanism of the physical world based on the principles of mechanics and thermodynamics. It aims to help students appreciate the beauty of physics and enable them to apply key concepts learnt to evaluate and address physics-based problems to make a positive impact on the world. By using concepts established through simplified mathematical models, reverse engineering case studies and experiential learning through hands-on demonstrations, connections between physics concepts and theoretical models are reinforced with practice.

● REFERENCES

Prof. Ir. Dr. Chai Siang Piao

Deputy Head of School (Research)
School of Engineering
Monash University Malaysia
47500 Subang Jaya
Tel: +603 5514 6234
Email: chai.siang.piao@monash.edu

Prof. Dr. Nikhil V. Medhekar

Department of Materials Science and Engineering
Faculty of Engineering
Monash University Clayton
Victoria 3800
Tel: +613 990 51421
Email: Nikhil.Medhekar@monash.edu

A/Prof. Dr. Ng Boon Junn

Assistant Professor
School of Energy and Chemical Engineering
Xiamen University Malaysia
Jalan Sunsuria, Bandar Sunsuria, 43900 Sepang,
Selangor, Malaysia
Tel: N/A.
Email: boonjunn.ng@xmu.edu.my