

## **Letter of Motivation from Dr. Jun Cheng for Chair of Division 7**

The International Society of Electrochemistry (ISE) is one of the most important and influential organizations that serve the broad electrochemistry community to promote education, research, science and technology in the field of electrochemistry. I was first introduced to the ISE by Prof. Marc Koper at Leiden in 2014. He kindly invited me to give a lecture in the 65<sup>th</sup> ISE annual meeting in Lausanne. At that time, I just started my independent position at Aberdeen, trying to set up my group and find ways to model complex electrochemical interfaces. The ISE meeting offered me a great platform to promote my research to the community and a valuable opportunity to exchange ideas and thoughts with experimental and theoretical electrochemists in the related areas. Soon later, I published my first paper in *Electrochimica Acta*.

During my research career, I was helped by the senior members of the society and benefited by the meetings and journals sponsored by the society. I am therefore excited about the opportunity to serve the community and contribute to the operation of the society.

On the other hand, if working as a division officer, I would be able to engage with the broader community, and interact with a wider number of the ISE members. In order to propose symposia topics, I would need to develop a broad view of various related research areas to identify hot topics of broad interest to the society. There are also opportunities to contribute to a long term scientific planning within the society by setting up priority options. If elected as a division officer, fulfillment of the duties would help me broaden my research perspective, identify emerging research themes, and establish potential collaborations with other members.

Finally, I have education background and research experience in both China and UK, and am familiar with academic systems at both sides. I am therefore in a good position to help bring together the electrochemists in Europe and Asia, and better serve the whole society at an international level.

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## Education

2005-2008 Ph.D. in Theoretical Chemistry, Queen's University Belfast  
2002-2005 M.ENG. in Chemical Engineering, Shanghai Jiao Tong University  
1998-2002 B.Sc. in Chemistry, Shanghai Jiao Tong University

## Employment

2013- PROFESSOR, College of Chemistry and Chemical Engineering, Xiamen University, China  
2013-2015 UNIVERSITY LECTURER, Department of Chemistry, University of Aberdeen, UK  
2010-2013 JUNIOR RESEARCH FELLOW, Emmanuel College, University of Cambridge, UK  
2008-2010 RESEARCH ASSOCIATE, Department of Chemistry, University of Cambridge, UK

## Research interests

*Ab initio* electrochemistry    Theoretical catalysis    Energy materials    Machine learning

## Honors & awards

2024 Program for High-Level Talents, Fujian Province (A Class)  
2022 National Science Fund for Distinguished Young Scholars  
2021 Alexander Kuznetsov Prize for Theoretical Electrochemistry, the International Society of Electrochemistry  
2019 Chinese National Electrochemistry Youth Award  
2018 Zhao-Wu Tian Cross-Disciplinary Award, Xiamen University (First Prize)  
2015 "Minjiang Scholar" Distinguished Professor, Fujian Province  
2015 Overseas High-Level Talent Recruitment Programs  
2010-2013 Junior Research Fellowship, Emmanuel College, University of Cambridge

## Academic services

2022- Associate Editor of Journal of Chemical Physics  
2017- Associate Editor of Journal of Electrochemistry  
2020- Member of the Editorial Advisory Board of Chemical Physics Reviews  
2019- Member of the Early Career Advisory Board of ACS Catalysis  
2019- Member of the Publication Committee of the International Society of Electrochemistry

## Grants

2022 NSFC grant for Distinguished Young Scholars, China (PI: RMB 4 Million)  
2022 Huawei research grant, China (PI: RMB 1.7 Million)  
2021 NSFC grant, China (PI: RMB 770 Thousand)  
2020 NSFC innovation group program, China (Co-I: RMB 10 Million)  
2019 NSFC major grant, China (PI: RMB 4.8 Million)  
2019 XMU-PCOSS major grant, China (PI: RMB 3 Million)  
2018 Sino-German joint research project (PI with Prof. K. Reuter at TUM: RMB 1.3 Million)

2017 NSFC grant, China (PI: RMB 750 Thousand)  
2015 Oversea young talents recruiting program, China (PI: RMB 3 Million)  
2014 EPSRC Starting Grant, UK (PI: GBP 130 Thousand)  
2014 Leverhulme Trust Grant, UK (Co-I: GBP 69 Thousand)

## Selected publications

### BOOK CHAPTERS

- 2021 2. **Jun Cheng\***, et al., *Ab initio* modeling of semiconductor-water interfaces, in *Springer Handbook of Inorganic Photochemistry*, Springer.
- 2021 1. **Jun Cheng\***, et al., *Ab initio* modeling of electrochemical interfaces and determination of electrode potentials, in *Atomic-Scale Modelling of Electrochemical Systems*, John Wiley.

### JOURNAL ARTICLES

Full list of publications can be found in [Google Scholar](#)

Over 181 papers with 12977 citations, and H-index = 61 till August 2024

- 2024 30. Y. Sun, C.-R. Wu, F. Wang, R.-H. Bi, Y.-B. Zhuang, S. Liu, M.-S. Chen, K. H. L. Zhang\*, J.-W. Yan\*, B.-W. Mao, Z.-Q. Tian, **Jun Cheng\***  
Step-induced double-row pattern of interfacial water on rutile TiO<sub>2</sub>(110) at electrochemical conditions  
*Chem. Sci.*, 2024, 15, 12264-12269
- 2024 29. F. Wang, Z. Ma, **Jun Cheng\***  
Accelerating Computation of Acidity Constants and Redox Potentials for Aqueous Organic Redox Flow Batteries by Machine Learning Potential-Based Molecular Dynamics  
*J. Am. Chem. Soc.*, 2024.
- 2024 28. F.-Q. Gong, Y.-P. Liu, Y. Wang, W. E., Z.-Q. Tian, **Jun Cheng\***  
Machine Learning Molecular Dynamics Shows Anomalous Entropic Effect on Catalysis via Surface Pre-melting of Nanoclusters  
*Angew. Chem. Int. Ed.*, 2024, e202405379.
- 2023 27. F. Wang, Y. Sun, **Jun Cheng\***  
Switching of redox levels leads to high reductive stability in water-in-salt electrolytes  
*J. Am. Chem. Soc.*, 2023, 145, 4056-4064.
- 2022 26. F. Wang, **Jun Cheng\***  
Unraveling the origin of reductive stability of super-concentrated electrolytes from first principles and unsupervised machine learning  
*Chem. Sci.*, 2022, 13, 11570-11576.
- 2022 25. M. Lin, J. Xiong, M. Su, F. Wang, X. Liu, Y. Hou, R. Fu, Y. Yang\*, **Jun Cheng\***  
A machine learning protocol for revealing ion transport mechanisms from dynamic NMR shifts in paramagnetic battery materials  
*Chem. Sci.*, 2022, 13, 7863-7872.
- 2022 24. J. Kang, Q.-Y. Fan, W. Zhou, Q. Zhang, S. He, L. Yue, Y. Tang, L. Nguyen, X. Yu, Y. You, H. Chang, X. Liu, L. Chen, Y. Liu, F. Tao\*, **Jun Cheng\***, Y. Wang\*  
Iridium boosts the selectivity and stability of cobalt catalysts for syngas to liquid fuels  
*Chem.*, 2022, 8, 1050-1066.
- 2021 23. J.-B. Le, A. Chen, L. Li, J.-F. Xiong, J. Lan, Y.-P. Liu, M. Iannuzzi, **Jun Cheng\***  
Modeling Electrified Pt(111)-H<sub>ad</sub>/Water Interfaces from Ab Initio Molecular Dynamics  
*JACS Au*, 2021, 1, 569-577.
- 2021 22. J.-X. Huang, L.-F. Zhang, H. Wang, J.B. Zhao, **Jun Cheng\***, W.N. E  
Deep potential generation scheme and simulation protocol for the Li<sub>10</sub>GeP<sub>2</sub>S<sub>12</sub>-type superionic conductors  
*J. Chem. Phys.*, 2021, 154, 094703.
- 2021 21. M. Lin#, X. Liu#, Y. Xiang, F. Wang, Y. Liu, R. Fu, **Jun Cheng\***, Y. Yang\*  
Unravelling the fast alkali-ion dynamics in paramagnetic battery materials combined with NMR and deep-potential molecular dynamics simulation  
*Angew. Chem.*, 2021, 133, 12655-12661.

2021

20. H. Zheng, Y. Lu, K.-H. Ye, J. Hu, S. Liu, J. Yan, Y. Ye, Y. Guo, Z. Lin, **Jun Cheng\***, Y. Cao\*  
Atomically thin photoanode of InSe/graphene heterostructure  
*Nature Commun.*, **2021**, *12*, 91.
- 2020 19. J.-B. Le, Q.-Y. Fan, J.-Q. Li, **Jun Cheng\***  
Molecular origin of negative component of Helmholtz capacitance at electrified Pt(111)/water interface  
*Science Advances*, **2020**, *6*, eabb1219.
- 2020 18. X. Wu, J. Li, S. Xie, P. Duan, H. Zhang, J. Feng, Q. Zhang\*, **Jun Cheng\***, Y. Wang\*  
Selectivity Control in Photocatalytic Valorization of Biomass-Derived Platform Compounds by Surface Engineering of Titanium Oxide  
*Chem*, **2020**, *6*, 1.
- 2020 17. Y. Giret\*, P. Guo, L.-Feng Wang, **Jun Cheng\***  
Theoretical study of kinetics of proton coupled electron transfer in photocatalysis  
*J. Chem. Phys.*, **2020**, *152*, 124705. (2020 *JCP Editors' Choice*)
- 2020 16. W. Ma, S. Xie, T. Liu, Q. Fan, J. Ye, F. Sun, Z. Jiang, Q. Zhang\*, **Jun Cheng\***, Y. Wang\*  
Electrocatalytic reduction of CO<sub>2</sub> to ethylene and ethanol through hydrogen-assisted C–C coupling over fluorine-modified copper  
*Nature Catal.*, **2020**, *3*, 478.
- 2020 15. C. Chen, X. Zhu, X. Wen, Y. Li\*, **Jun Cheng\***, Q. Liu\*, J. Chen\*, S. Wang\*, *et al.*  
Coupling N<sub>2</sub> and CO<sub>2</sub> in H<sub>2</sub>O to synthesize urea under ambient conditions  
*Nature Chem.*, **2020**, *12*, 717.
- 2020 14. P. Xiong, H.-B. Zhao, X.-T. Fan, L.-H. Jia, H. Long, P. Xu, Z.-J. Liu, Z.-J. Wu, **Jun Cheng\***, H.-C. Xu\*  
Site-selective electrooxidation of methylarenes to aromatic acetals  
*Nature Commun.*, **2020**, *11*, 2706.
- 2019 13. J.-J. Sun, **Jun Cheng\***  
Solid-to-liquid phase transitions of sub-nanometer clusters enhance chemical transformation  
*Nature Commun.*, **2019**, *10*, 5400.
- 2019 12. C.-Y. Li, J.-B. Le, Y.-H. Wang, S. Chen, Z.-L. Yang, J.-F. Li\*, **Jun Cheng\***, Z.-Q. Tian  
In situ probing electrified interfacial water structures at atomically flat surfaces  
*Nature Mater.*, **2019**, *18*, 697.
- 2019 11. Y.-H. Wang, J.-B. Le, W.-Q. Li, J. Wei, P. M. Radjenovic, H. Zhang, X.-S. Zhou\*, **Jun Cheng\***, Z.-Q. Tian, J.-F. Li\*  
In situ Spectroscopic Insight into the Origin of the Enhanced Performance of Bimetallic Nanocatalysts towards the Oxygen Reduction Reaction (ORR)  
*Angew. Chem. Int. Ed.*, **2019**, *131*, 16208.
- 2019 10. X. Huang, C. Tang, J. Li, L. Chen, J. Liu\*, **Jun Cheng\***, Z.-Q. Tian, W. Hong\*, *et al.*  
Electric field-induced selective catalysis of single-molecule reaction  
*Science Advances*, **2019**, *5*, eaaw3072.
- 2019 9. X.-J. Zhao, H. Hou, X.-T. Fan, **Jun Cheng\***, Y.-Z. Tan\*, *et al.*  
Molecular bilayer graphene  
*Nature Commun.*, **2019**, *10*, 3057.
- 2018 8. X.-J. Wu, X.-T. Fan, S. Xie, J. Lin, **Jun Cheng\***, Q.-H. Zhuang\*, L. Chen, Y. Wang\*  
Solar energy-driven lignin-first approach to full utilization of lignocellulosic biomass under mild conditions  
*Nature Catal.*, **2018**, *1*, 772.
- 2018 7. S. Xie, Z. Shen, J. Deng, P. Guo, Q. Zhang, H. Zhang, C. Ma, Z. Jiang, **Jun Cheng\***, D. Deng\*, Y. Wang\*  
Visible light-driven C–H activation and C–C coupling of methanol into ethylene glycol  
*Nature Commun.*, **2018**, *9*, 1181.
- 2017 6. B. An, L. Zeng, M. Jia, Z. Li, Z. Lin, Y. Song, Y. Zhou, **Jun Cheng\***, C. Wang\*, W. Lin\*  
Molecular Iridium Complexes in Metal–Organic Frameworks Catalyze CO<sub>2</sub> Hydrogenation via Concerted Proton and Hydride Transfer  
*J. Am. Chem. Soc.*, **2017**, *139*, 17747.
- 2017 5. J. Le, M. Iannuzzi, A. Cuesta, **Jun Cheng\***  
Determining potentials of zero charge of metal vs standard hydrogen electrode from density functional theory based molecular dynamics  
*Phys. Rev. Lett.*, **2017**, *119*, 016801.
- 2016 4. **Jun Cheng\***, J. VandeVondele\*  
Calculation of electrochemical energy levels in water using the random phase approximation and

a double hybrid functional

*Phys. Rev. Lett.*, **2016**, *116*, 086402.

2014 3. **Jun Cheng\***, X. Liu, J. VandeVondele, M. Sulpizi, M. Sprik\*  
Redox potentials and acidity constants from ab initio molecular dynamics

*Acc. Chem. Res.*, **2014**, *47*, 3522-3529.

2014 2. **Jun Cheng\***, X. Liu, J. A. Kattirtzi, J. VandeVondele, M. Sprik  
Aligning electronic and protonic energy levels of proton coupled electron transfer in water oxidation on aqueous TiO<sub>2</sub>

*Angew. Chem. Int. Ed.*, **2014**, *53*, 12046-12050. (*Frontispecies*)

2014 1. Y.-K. Lv, **Jun Cheng\***, A. Steiner, L. Gan, D. S. Wright\*  
Dipole-induced Band Gap Reduction in an Inorganic Cage

*Angew. Chem. Int. Ed.*, **2014**, *126*, 1965-1969.

## Selected talks

2024 Invited talk, MRS 2024 Fall Meeting, Symposium "Recent Advancements in Characterization and Modeling of Electrochemical Interfaces", Boston, MA, USA

2024 Invited talk, ECS PRiME 2024, Honolulu, Hawaii, USA.

2024 Invited talk, the 6th Materials Chain International Conference (MCIC 2024), Bochum, Germany

2024 Invited talk, the 38th Topical Meeting of the International Society of Electrochemistry on the Electrochemistry of Nanomaterials, Manchester, UK

2024 Invited talk, the 75th Annual Meeting of the International Society of Electrochemistry, Montreal, Canada

2024 Invited talk, International Symposium on Electrochemistry and Surface Science in Honour of Professor Jacek Lipkowski's 80th Birthday, Ontario, Canada

2024 Invited talk, Lorentz Center workshop on opportunities and challenges in the multiscale modeling of electrochemical processes, Leiden, the Netherlands

2024 Invited talk, Marcus Wallenberg Symposium on Metal-Oxide/Water Interactions in Electrochemistry (MOWiiE), Uppsala, Sweden

2024 Invited talk, the 14th International Workshop on Oxide Surfaces, IWOX-14, Schladming, Austria.

2023 Invited talk, the 6th China-Japan-Korea Workshop on Theoretical and Computational Chemistry (CJK-WTCC-VI), Suwon, South Korea.

2023 Invited talk, 4th Southeast Asia Catalysis Conference (SACC), Singapore.

2022 Invited talk, the International Workshop "Electrified solid/water interfaces – theory meets experiment", Ringberg Castle, Tegernsee, Germany.

2022 Invited talk, the CECAM flagship workshop: Recent Advances in Machine Learning Accelerated Molecular Dynamics, Pisa, Italy.

2021 Invited talk, ICTP Workshop on Physics and Chemistry of Solid/Liquid Interfaces for Energy Conversion and Storage, the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy.

2021 Keynote talk, the online nanoGe Spring Meeting 2021: Solar fuels.

2020 Invited talk, the 6th International Conference on Electronic Materials and Nanotechnology for Green Environment ENGE 2020, Jeju, South Korea.

2020 Invited talk, Catalysis in time of Coronavirus – An online webinar series, Catalysis Theory Centre, DTU, Denmark.

2019 Invited talk, Operando Surface Science – Atomistic Insights into Electrified Solid/liquid Interfaces, the 708. WE-Heraeus-Seminar, Physikzentrum Bad Honnef, Germany.

2019 Invited talk, the 70th Annual Meeting of the International Society of Electrochemistry, Durban, South Africa.

2018 Invited lecture, Swiss Symposium and Summer School 2018: Solar Light to Chemical Energy Conversion, Les Diablerets, Switzerland.

2018 Invited talk, Simulations (and Theory) in Physical Chemistry: an International Kermesse in Paris, Paris, France.

2017 Invited talk, The Electrode Potential in Electrochemistry – A Challenge for Electronic Structure Theory Calculations, a Workshop at Castle Reisenburg, Ulm, Germany.

2017 Invited talk, The CPMD 2017 meeting, Tsukuba, Japan.

2017 Invited talk, the 68th Annual Meeting of the International Society of Electrochemistry, Providence, RI, USA.