

Dr. Xue Yong

Lecturer in Computational Chemistry

Leverhulme Early Career Fellow

University of Liverpool, UK

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Research Expertise

- First-principles modelling (DFT, AIMD) of dynamic electrocatalysts and energy-conversion materials
- Physics-informed and interpretable machine learning for catalyst design
- Electrochemical conversion of nitrogen-, carbon-, oxygen-, and hydrogen-containing species
- Sustainable aviation fuel development and molecular-property screening
- Design of transport and optical functional materials

Academic Appointments

Lecturer in Computational materials University of Liverpool, UK	2024–present
Leverhulme Early Career Fellow University of Liverpool, UK	2024–2026
Leverhulme Early Career Fellow University of Sheffield, UK	2021–2024
NSERC PDF University of Calgary, Canada	2019–2021
Scientist I Institute of High Performance Computing, ASTAR, Singapore	2016–2019

Education

Ph.D. Physics & Engineering Physics University of Saskatchewan, Canada	2012–2017
M.Sc. Physical Chemistry Northeast Normal University, China Thesis: <i>Design strategies for organic solar cell donor materials (first-principles calculations)</i>	2009–2012
B.Sc. Chemistry Northeast Normal University, China	2005–2009

Grants & Fellowships

- Leverhulme Early Career Fellowship (£158K, PI, 2023–2026): Computational characterisation of carbon dots
- EPSRC Supergen Hub – Smart Catalysts for Smart Grids (£100K, PI, 2026–2027) UKRI HPC access, Computational Design catalyst for biomass upgrading (PI, 2024–2025)
- University of Liverpool-Taiwan dual PhD studentship (PI, 2026–2030)
- University of Sheffield PhD Studentship – Sustainable aviation fuel datasets (£90K, PI, 2023–2027)
- Fusion CDT Project – Fusion reactor wall materials (£100K, PI, 2025–2029)
- British Council – Feed the Future Programme (£5K, PI, 2024–2025)
- NSERC Postdoctoral Fellowship (PI, 2021–2022): High-pressure helium chemistry

Publications

- [1] Syarir Akram Bin Jamaluddin, **Xue Yong***, Ehsan Alborzi, Gary Dunderdale, and Mohamed Pourkashanian. Constructing a novel dataset for permittivity and density of hydrocarbon classes in the range of aviation fuels via molecular dynamic simulations and experiments. *Fuel* 405 (2026), p. 136738.
- [2] Yaojia Cheng, Tingting Zhai, **Xue Yong**, Ran Zhang, Dan Pan, Yongjuan Yuan, Zhiyong Tang, Hao Wang, and Siyu Lu. Grain-boundary-rich Mo-doped RuO₂ for highly efficient and stable proton-exchange-membrane water electrolysis. *ACS nano* 19.38 (2025), pp. 34329–34340.

- [3] Yue Feng, Yuzhuo Cai, Yaolin Wang, Tianyu Li, Santu Luo, Wenpeng Liang, Sutao Zheng, Tao Xie, Qing-Yuan Yang, **Xue Yong**, et al. Enhanced ammonia synthesis using surface microdischarge with metal-loaded nickel foam electrodes. *Chemical Engineering Journal* 510 (2025), p. 161553.
- [4] Zhiang Hu, Han Wu, **Xue Yong**, Geoffrey IN Waterhouse, Zhiyong Tang, Junbiao Chang, Jiangwei Chang, and Siyu Lu. Advances in dual-site mechanisms for designing high-performance oxygen evolution electrocatalysts. *eScience* (2025), p. 100403.
- [5] Ting-Ting Shen, Jing Liu, Fang-Yuan Bai, Wei-Wei Xu, **Xue Yong**, Zhi-Rong Li, Jing-Ru Han, Jun Chen, Heng Zhao, Zhi-Yi Hu, et al. Regulating the band gap of $Zn_xCd_{1-x}S$ in 3DOM $CaTiO_3$ for high hydrogen evolution and gluconic acid selectivity. *Inorganic Chemistry Frontiers* (2025).
- [6] Wei Wang, Minh Nguyen-Quang, Diego Mateo, **Xue Yong**, Tao Li, Haiquan Xie, Wei Chu, Cuong Pham-Huu, Xin Tu, and Jorge Gascon. A Review of CO_2 Methanation Process: Recent Advances and Future Prospects. *ACS Catalysis* 15 (2025), pp. 10868–10896.
- [7] Han Wu, Zhanzhao Fu, Jiangwei Chang, Zhiang Hu, Jian Li, Siyang Wang, Jingkun Yu, **Xue Yong**, Geoffrey IN Waterhouse, Zhiyong Tang, et al. Engineering high-density microcrystalline boundary with V-doped RuO_2 for high-performance oxygen evolution in acid. *Nature Communications* 16.1 (2025), p. 4482.
- [8] Jingkun Yu, **Xue Yong***, and Siyu Lu. $Li_{10}Bi$: A Lithium-Rich Electride with Coexisting Superconductivity and Solid-State Lithium-Ion Conductivity. *Chinese Physics B* (2025).
- [9] Jingkun Yu, **Xue Yong***, Siyu Lu, and John S Tse. Hydrogen-Based Superconductors: Superconducting Mechanisms under Pressure Tuning and Future Development. *Chinese Journal of Chemistry* 43.24 (2025), pp. 3699–3715.
- [10] Man Zhang, Zhikeng Zheng, Xiaodie Zhang, Zhiwei Jiang, **Xue Yong**, Ke Li, Xin Tu, and Kai Yan. Pairing electrocatalytic reduction and oxidation of biomass-derived 5-hydroxymethylfurfural into highly value-added chemicals. *JACS Au* 5.2 (2025), pp. 937–947.
- [11] Yuan Zhao, Hanqi Yu, Jiuchao Tang, Yingmei Li, **Xue Yong***, Xin Tu, and Jing Wang. Strain engineering of heterogeneous catalysts for oxygen reduction reaction. *Chinese Chemical Letters* (2025), p. 111997.
- [12] Charlie Adams, Ehsan Alborzi, **Xue Yong**, Simon Blakey, Anthony JHM Meijer, and Mohamed Pourkashanian. Experimental and quantum chemical investigation into the nature of jet fuel deposition on surfaces. *Fuel* 358 (2024), p. 130101.
- [13] Ehsan Alborzi, **Xue Yong**, Morteza Roostaeinia, Detlev C Mielczarek, Irina S Flyagina, Simon G Blakey, and Mohamed Pourkashanian. Effect of Zeolite 3.7 A coated monoliths on improvement of aviation fuel thermal oxidative stability. *Fuel* 360 (2024), p. 130498.
- [14] Ana M Garrote Canas, **Xue Yong**, Maha S Alenezi, Natalia Martinsovich, and Natalia N Sergeeva. Phenanthrolines decorated with branched lipophilic chains and their yellow emitting heteroleptic iridium (III) complexes: Synthesis, photophysical and acidochromic behaviour, and computational analysis. *Dyes and Pigments* 222 (2024), p. 111844.
- [15] Jiangwei Chang, Wen Jing, **Xue Yong**, Ang Cao, Jingkun Yu, Han Wu, Chengzhang Wan, Siyang Wang, Geoffrey IN Waterhouse, Bai Yang, et al. Synthesis of ultrahigh-metal-density single-atom catalysts via metal sulfide-mediated atomic trapping. *Nature Synthesis* 3.11 (2024), pp. 1427–1438.
- [16] Henghui Chen, Jing Wang, Yuan Zhao, Xufeng Zhou, Heran Yang, Yan Li, Yingmei Li, Ehsan Alborzi, **Xue Yong**, and John S Tse. Interface engineering of the d_{z^2} electrons mobility for single atom catalytic activity and selectivity. *Materials Today Energy* 45 (2024), p. 101661.
- [17] Junpeng Chen, Jing Wang, Shuang Li, Yuan Zhao, Jiachao Zhao, Xinyu Liang, Meirong Xia, Yingmei Li, Jun Yang, **Xue Yong***, et al. Co-NC axially coordination regulated H_2O_2 selectivity via water mediated recombination of solute $\cdot OH$: A new route. *Chemical Engineering Journal* 489 (2024), p. 151412.
- [18] Jiao-Zi Duan, Hua-Yu Pei, Quan Yang, Xu Li, Xin Ba, **Xue Yong**, Jun-Ling Guo, and Si-Yu Lu. Carbon dots-derived three-dimensional-ordered macroporous host with high penetrability and catalytic activity for LSBs under lean electrolyte. *Rare Metals* 43.6 (2024), pp. 2560–2573.
- [19] Bingqiu Liu, Qi Zhang, Lingyu Zhang, **Xue Yong**, Lu Li, and Chungang Wang. Manganese charge redistribution induced by high-entropy charge compensation mechanism for aqueous potassium-ion batteries. *Energy Storage Materials* 66 (2024), p. 103221.
- [20] Yaru Shang, Tianxing Liu, Gang Chen, Ehsan Alborzi, **Xue Yong**, and Yu Wang. N, P co-doped carbon quantum dots bridge $g-C_3N_4$ and SnO_2 : Accelerating charge transport in S-scheme heterojunction for enhanced photocatalytic hydrogen production. *Journal of Alloys and Compounds* 971 (2024), p. 172667.
- [21] Haoqiang Song, **Xue Yong**, Geoffrey IN Waterhouse, Jingkun Yu, Hao Wang, Jinqiang Cai, Zhiyong Tang, Bai Yang, Jiangwei Chang, and Siyu Lu. RuO_2-CeO_2 lattice matching strategy enables robust water oxidation electrocatalysis in acidic media via two distinct oxygen evolution mechanisms. *Acs Catalysis* 14.5 (2024), pp. 3298–3307.

- [22] Han Wu, Jiangwei Chang, Jingkun Yu, Siyang Wang, Zhiang Hu, Geoffrey IN Waterhouse, **Xue Yong**, Zhiyong Tang, Junbiao Chang, and Siyu Lu. Atomically engineered interfaces inducing bridging oxygen-mediated deprotonation for enhanced oxygen evolution in acidic conditions. *Nature Communications* 15.1 (2024), p. 10315.
- [23] Jingkun Yu, **Xue Yong**, Ang Cao, and Siyu Lu. Bi-layer single atom catalysts boosted nitrate-to-ammonia electroreduction with high activity and selectivity. *Acta Physico-Chimica Sinica* 40.6 (2024). Corresponding author, p. 2307015.
- [24] Jingkun Yu, **Xue Yong***, Hanyu Liu, and Siyu Lu. Prediction of enhanced superconductivity in cyclo-H₁₂ Bi/Pb involving a resonant hydrogen structure. *Physical Review B* 110.22 (2024), p. 224507.
- [25] Jingkun Yu, **Xue Yong***, and Siyu Lu. p-d orbital hybridization engineered single-atom catalyst for electrocatalytic ammonia synthesis. *Energy & Environmental Materials* 7.2 (2024), e12587.
- [26] Xuchu Yuan, Jintao Sun, Yichen Ma, Yaolin Wang, Bowen Liu, Yuxiang Cai, **Xue Yong**, and Xin Tu. A kinetic study of nonthermal plasma pyrolysis of methane: Insights into hydrogen and carbon material production. *Chemical Engineering Journal* 499 (2024), p. 156396.
- [27] Baowei Zhang, Yi Ru, Jiaqian Zhou, Jingtao Jia, Haoqiang Song, Zhongyi Liu, Linlin Zhang, Xuying Liu, Guiming Zhong, **Xue Yong**, et al. A Robust Anti-Thermal-Quenching Phosphor Based on Zero-Dimensional Metal Halide Rb₃InCl₆: x Sb³⁺. *Journal of the American Chemical Society* 146.11 (2024), pp. 7658–7667.
- [28] Lin Ai, Yifei Pei, Ziqi Song, **Xue Yong**, Haoqiang Song, Gongjie Liu, Mingjun Nie, Geoffrey IN Waterhouse, Xiaobing Yan, and Siyu Lu. Ligand-triggered self-assembly of flexible carbon dot nanoribbons for optoelectronic memristor devices and neuromorphic computing. *Advanced Science* 10.12 (2023), p. 2207688.
- [29] Tengfei Liu, Guangchao Yin, Ziqi Song, Jingkun Yu, **Xue Yong**, Baowei Zhang, Lin Ai, and Siyu Lu. Solid-state luminescence in self-assembled chlorosalicylaldehyde-modified carbon dots. *ACS Materials Letters* 5.3 (2023), pp. 846–853.
- [30] Yi Ru, Baowei Zhang, **Xue Yong**, Laizhi Sui, Jingkun Yu, Haoqiang Song, and Siyu Lu. Full-color circularly polarized luminescence of CsPbX₃ nanocrystals triggered by chiral carbon dots. *Advanced Materials* 35.5 (2023), p. 2207265.
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- [32] Haolin Wang, Lin Ai, Haoqiang Song, Ziqi Song, **Xue Yong**, Songnan Qu, and Siyu Lu. Innovations in the solid-state fluorescence of carbon dots: strategies, optical manipulations, and applications. *Advanced Functional Materials* 33.41 (2023), p. 2303756.
- [33] Yixuan Wang, Chuang Liu, **Xue Yong**, Xinyi Yang, Jingkun Yu, Siyu Lu, Fuquan Bai, Shiping Wang, Kai Wang, Zhaodong Liu, et al. Pressure engineering toward harvesting the bright deep-blue-light emission in Y-based metal-organic frameworks. *Advanced Functional Materials* 33.21 (2023), p. 2300109.
- [34] **Xue Yong**, Thiba Nagaraja, Rajavel Krishnamoorthy, Ana Guanes, Suprem R Das, and Natalia Martsinovich. Theoretical and experimental studies of molecular interactions between engineered graphene and phosphate ions for graphene-based phosphate sensing. *ACS Applied Nano Materials* 7.16 (2023), pp. 18386–18397.
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- [36] Dafeng Zhang, Mengnan Li, **Xue Yong***, Haoqiang Song, Geoffrey IN Waterhouse, Yunfei Yi, Bingjie Xue, Dongliang Zhang, Baozhong Liu, and Siyu Lu. Construction of Zn-doped RuO₂ nanowires for efficient and stable water oxidation in acidic media. *Nature Communications* 14.1 (2023), p. 2517.
- [37] Ting Zhang, **Xue Yong**, Jingkun Yu, Yixuan Wang, Min Wu, Qing Yang, Xuyuan Hou, Zhaodong Liu, Kai Wang, Xinyi Yang, et al. Brightening blue photoluminescence in nonemission MOF-2 by pressure treatment engineering. *Advanced Materials* 35.23 (2023), p. 2211729.
- [38] Heng Zhao, Dhwanil Trivedi, Morteza Roostaenia, **Xue Yong**, Jun Chen, Pawan Kumar, Jing Liu, Bao-Lian Su, Steve Larter, Md Golam Kibria, et al. Spatial charge separation on the (110)/(102) facets of cocatalyst-free ZnIn₂S₄ for the selective conversion of 5-hydroxymethylfurfural to 2, 5-diformylfuran. *Green Chemistry* 25.2 (2023), pp. 692–699.
- [39] Hong-Wen Liang, Tian Jia, **Xue Yong**, Jing-Kun Yu, Yu Yi, Siyu Lu, Lei Wang, and Hao Wang. Photoinduced single-crystal to single-crystal transformation via conformational change with turn-on fluorescence. *Crystal Growth & Design* 22.4 (2022), pp. 2082–2086.
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- [42] Zicong Marvin Wong, **Xue Yong**, Tianqi Deng, Wen Shi, Gang Wu, Ning Li, He-Kuan Luo, and Shuo-Wang Yang. Neutral Antiaromatic Bis (1, 2-dithiolene)-Chelated Nickel Complexes Bearing Multiradical Characters. *The Journal of Physical Chemistry A* 126.33 (2022), pp. 5552–5558.
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- [48] Ali Naderi, **Xue Yong**, Mohammadreza Karamad, Jinyan Cai, Yipeng Zang, Ian Gates, Samira Siahrostami, and Gongming Wang. Ternary cobalt–iron sulfide as a robust electrocatalyst for water oxidation: a dual effect from surface evolution and metal doping. *Applied Surface Science* 542 (2021), p. 148681.
- [49] Meng-En Sun, Ting Geng, **Xue Yong**, Siyu Lu, Lin Ai, Guanjun Xiao, Jinmeng Cai, Bo Zou, and Shuang-Quan Zang. Pressure-Triggered Blue Emission of Zero-Dimensional Organic Bismuth Bromide Perovskite. *Advanced Science* 8.9 (2021), p. 2004853.
- [50] Zhen-Yu Wu, Mohammadreza Karamad, **Xue Yong**, Qizheng Huang, David A Cullen, Peng Zhu, Chuan Xia, Qunfeng Xiao, Mohsen Shakouri, Feng-Yang Chen, et al. Electrochemical ammonia synthesis via nitrate reduction on Fe single atom catalyst. *Nature communications* 12.1 (2021), p. 2870.
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- [53] Tianqi Deng, **Xue Yong**, Wen Shi, Zicong Marvin Wong, Gang Wu, Hui Pan, Jian-Sheng Wang, and Shuo-Wang Yang. Beyond the Mahan–Sofo best thermoelectric strategy: high thermoelectric performance from directional π -conjugation in two-dimensional poly (tetrathienoanthracene). *Journal of Materials Chemistry A* 8.8 (2020), pp. 4257–4262.
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Teaching Experience

- University of Liverpool: ELEC191 – Mathematics A for Electrical Engineers (2024, 2025)
- University of Sheffield: Computational Chemistry Laboratory (2021)
- University of Sheffield: Mathematics for Chemists (2022)

Supervision & Mentoring

- Academic Advisor to 20 undergraduate students
- Supervisor: 2 postdocs, 4 PhD (primary), 6 PhD (co-supervisor), 7 final-year projects, 1 MSc

Professional Service & Memberships

- Member of Royal Society of Chemistry (2023–present)
- Committee Member, British Carbon Group (2025–present)
- Committee Member, Royal Society Chemistry Energy Sector (2025–present)
- ECR board, Nano letter (2025-2028)

Award

- Leverhulme Early Career Fellowship (2023)
- NSERC Postdoctoral Fellowship (2019)
- Best Researcher Award (2024)