

Dr Yao Wei

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Research and Work Experience

Czech Academy of Sciences, CZ

Marie Skłodowska-Curie Actions (MSCA) COFUND Fellowship 2026—

Decarbon Journal (published by Elsevier)

Emerging Young Scholar Editorial Board Member 2026—

- Contribute to peer review, special-issue development, and strategic planning for the journal.

Slovak Academy of Sciences, SK

Senior Scientist Researcher 2025—2026

- Collaborator with: Ivan Stich
- Contribute to research projects: **VEGA 2/0133/25, Supercomputer modelling of 2D nanomaterials using first-principles methods with AI support.**
- Contracted to conduct research on condensed matter physics at the Institute of Informatics, Slovak Academy of Sciences. During the contract period, collaborated with the group on Quantum Monte Carlo (QMC). On-site appointment was not taken up owing to visa processing delays, following the award of a Marie Skłodowska-Curie Fellowship.

King's College London, UK

Graduate Teaching Associate & Research Associate 2020—08/2025

Rep of Staff Student Liaison Committee 2023—2024

The mentor of Success for Black Students Program 2024—08/2025

Visiting Researcher 08/2025—

- Supervised by: Lev Kantorovich, Jan Tomczak, Cedric Weber, Nicola Bonini.
- Lead tutorials for Physics Skills and Techniques, Numerical Modelling, Experimental Physics.
- Supervised 100+ students per semester, providing academic mentorship and grading assessments (coursework, reports, group projects).
- Collaborated with faculty to ensure course alignment with departmental and university standards.
- Acting as a bridge between students and academic staff, responsible for collecting student feedback, participating in departmental meetings, and contributing to the enhancement of teaching and learning within the department.
- Provided tailored academic and mental support to several Black students, assisting them with postgraduate applications, tutoring, and integration into the university community.
- Contribute to research projects: New Emergent Quantum States of Matter at High Pressure (Funded by the **EPSRC Engineering and Physical Sciences Research, UK, 2020–2022**).
- Research Content: The project is to propose a surface matrix (device) of high catalytic activity to specific chemical reactions, it would like to have clusters of metal atoms to be secured on a surface of some material, and then optimize the clusters composition such that to achieve their “best” catalytic activity to some simple chemical reactions like dissociation of CO, water, etc. This work should guide the experimentalists in terms of which metal atom numbers to be produced in their gun device to achieve the best catalytic activity for a chosen chemical reaction (Collaboration with Prof. Alessandro Baraldi at University of Trieste and Valera Veryazov at Lund University).

University of Cambridge, UK

2022—2024

Research Associate

- Supervised by: Bartomeu Monserrat.

- Contribute to research projects: Theoretical Condensed Matter - Critical Mass Grant (Funded by the **EPSRC Engineering and Physical Sciences Research, UK**, 2022–2026); Developed DMFT method for non-diagonal phonon calculations and applied it to high temperature and high-pressure superconducting materials (Collaboration with Prof. Samuel Ponce at UC Louvain).
- Research Content: It is possible to routinely solve the equations of quantum mechanics using density functional theory (DFT) to calculate the properties of many materials, such as silicon. However, DFT fails when considering materials hosting d and f electrons, so-called strongly correlated materials. In this case, more sophisticated methods, such as dynamical mean-field theory (DMFT) are required. In this project, the work on extending the applicability of DMFT to the calculation of phonons, which will enable the study of thermodynamic properties of strongly correlated materials.

Materials and Molecular Modelling Hub & Thomas Young Centre, UK

2023—2024

Activities & Conferences Co-organizer

- Prepared conference materials, liaised with participants, and arranged accessibility support.
- Observed academic proceedings to develop insights into scientific dialogue.
- Organized case files, drafted briefing documents, and coordinated schedules to ensure smooth event delivery.
- Managed the organization of several large-scale conferences, each with over 100 attendees.

Education

Ph.D. in Physics, King's College London, UK

10/2020—08/2025

- Sponsored by full PhD scholarship (2020-2025)
- PhD thesis: *Study of electronic and vibrational properties of some transition metal-containing materials with applications to catalysis and superconductivity*
- Research areas: Quantum mechanics, Condensed matter physics, Room Temperature Superconductivity, Dynamical Mean Field Theory, Quantum computing, Surface Defects and adsorbed species, Catalysis
- Award: King's Student Opportunity Fund (2022-2023) and Student Opportunity Fund (2023-2024)

Visiting Ph.D. in Computational Materials Science, University of Cambridge, UK

09/2022—07/2024

- Research areas: Extending the applicability of DMFT to the calculation of phonons, which will enable the study of thermodynamic properties of strongly correlated materials
- Award: American Physical Society (APS) Distinguished Student Program (DS) 2023

MSc, Electronic engineering with management, King's College London, UK

09/2018—01/2020

- Core Modules: Artificial Intelligence, Operations Research, Pattern Recognition
- Award: King's London Experience Award

Grants & Fellowships

- Physics for Future (P4F) Postdoctoral Fellowship (**Horizon Europe MSCA COFUND**, Grant No. 101081515). Institute of Physics of the Czech Academy of Sciences (FZU) & ELI Beamlines, Prague, Czech Republic (24 months) Prestigious EU-funded fellowship with full financial support totaling **€111,360 over 24 months** (includes employer contributions). Additional dedicated research, training and networking budget provided by the host institution for project costs, consumables, travel and open-science activities (2026-2028).
- POST-DOC/0925 - ROandOther (Cyprus RIF RESTART 2016–2020, SUPERCOND) — **Scored 13.35/15.00 (89%, Eligible)** by two independent evaluators; ranked top but not funded due to budget exhaustion. Excellence recognized in ab initio superconductivity, open-source tools, and international collaboration (submitted Nov 2025; evaluated Apr 2026).
- **Awarded access to 22 million CPUs on the Archer2 (UK's national supercomputer)** HPC facility, serving as the independent PI for this allocation (equivalent of ~ £ 65,000 funding) (2025).

- **Awarded access to 24 million CPUhs on the Archer2 (UK's national supercomputer)** HPC facility, serving as the independent PI for this allocation (equivalent of ~ £ 74,000 funding) (2024).
- **Awarded access to 2 million CPUhs on the Archer2 (UK's national supercomputer)** HPC facility, serving as the independent PI for this allocation (equivalent of ~ £ 8,190 funding) (2023).
- **Managed a project allocation of 22.5 million CPU core-hours** on the EPSRC-funded UK Materials and Molecular Modelling Hub (Young) throughout PhD research (2020–2025).
- **Full scholarship of Ph.D.** (2020-2025)

Media Coverage / Press Releases

- Featured in King's College London official news: “New method for predicting high-temperature superconducting materials” (19 January 2026). [Link](#)
- Featured on Thomas Young Centre official website: “Global Optimization of Molybdenum Subnanoclusters on Graphene: A Consistent Approach toward Catalytic Applications”. Highlighted the development of a PSO + ab initio global optimisation framework for subnanometer cluster catalysts, simulating experimental deposition and reactivity CO dissociation (Nov 2024) . [Link](#)

Technical Skills

- **Electronic Structure & Many-Body Methods:** VASP, WIEN2k, CP2K, Quantum ESPRESSO, EDMFTF (DMFT), CASTEP, PHONOPY, TDEP.
- **Programming & Scripting:** Python (NumPy, SciPy, ASE, Matplotlib), Bash

Publications

I. Journal Articles

- Chen S[#], **Wei Y[#]**, Monserrat B, et al. Impact of electronic correlations on the superconductivity of high-pressure CeH₉[J]. npj Computational Materials, 2026, 12(1): 32.
- **Wei Y[#]**, Chen S, Plekhanov E, et al. Correlation-driven phonon renormalisation and the equation of state of γ -cerium [J] (accepted by Physical Review B)
- **Wei Y**, Chen S, Monserrat B. Characterisation of spin–orbit effects in superconductors In₅Bi₃ and In₅Sb₃[J]. Journal of Physics: Materials, 2025, 8(2): 025015.
- Chachkarova E, Tse T, Yordanov Y, **Wei Y**, et al. Quantum Embedding of Non-Local Quantum Many-Body Interactions in an Prototypal Anti-Tumor Vaccine Metalloprotein on Near-Term Quantum Computing Hardware[J]. International Journal of Molecular Sciences, 2025, 26(4): 1550.
- **Wei Y**, Santana-Bonilla A, Kantorovich L. Global Optimization of Molybdenum Subnanoclusters on Graphene: A Consistent Approach toward Catalytic Applications[J]. ACS Applied Materials & Interfaces, 2024, 16(46): 64177-64189.
- **Wei Y**, Veryazov V, Kantorovich L. A comprehensive exploration of structural and electronic properties of molybdenum clusters[J]. APL Materials, 2024, 12(3). **(Selected as Editor's Pick)**
- **Wei Y**, Chachkarova E, Plekhanov E, et al. Exploring the Effect of the Number of Hydrogen Atoms on the Properties of Lanthanide Hydrides by DMFT[J]. Applied Sciences, 2022, 12(7): 3498.
- **Wei Y**, Macheda F, Zhao Z, et al. High-temperature superconductivity in the lanthanide hydrides at extreme pressures[J]. Applied Sciences, 2022, 12(2): 874.
- Plekhanov E, Zhao Z, Macheda F, **Wei Y**, et al. Computational materials discovery for lanthanide hydrides at high pressure for high temperature superconductivity[J]. Physical Review Research, 2022, 4(1): 013248.
- Zhao M, Zuo S, **Wei Y**, et al. Overview of structure and key problems for transverse flux permanent magnet linear machine [J]. Proceedings of the Chinese Society of Electrical Engineering, 2021, 41(22): 7806.

- **Wei Y**, Zhao M, Yang H, et al. Electromagnetic characteristic of a novel linear flux switching machine with three-dimensional magnetic circuit [J]. IEEE Transactions on Applied Superconductivity, 2019, 29(2): 1–5.
- Zhao M, **Wei Y**, Yu S, et al. Development and analysis of a novel transverse flux permanent magnet linear motor with the concentrated flux mover [J]. IEEE Transactions on Applied Superconductivity, 2019, 29(2): 1–6.
- Zhao M, **Wei Y**, Yang H, et al. Development and analysis of novel flux switching transverse flux permanent magnet linear machine [J]. IEEE Transactions on Industrial Electronics, 2019, 66(6): 4923–4933.

II. Conference Speech, Conference Papers and Posters

- **Wei Y**, “A comprehensive exploration of structural and electronic properties of Molybdenum clusters” *DPG Spring Meeting 2024 (Berlin, Germany)*. [Link](#)
- **Wei Y**, “Carbon, oxygen and carbon monoxide adsorption on graphene-supported size-selected Mo clusters” *MMM Hub Conference & User Meeting 2024 (London, UK)*. [Link](#)
- **Wei Y**, “Rational Design of Molybdenum Transition-Metal subnanoclusters catalysts with Particle Swarm Optimization” *TYC Postgraduate Student Day 2024 (London, UK)*. [Link](#)
- **Wei Y**, “Superconductivity of cerium hydride at high pressure from DFT+DFPT+DMFT” *APS March Meeting 2023 (Las Vegas, USA)*. [Link](#)
- **Wei Y**, “Global Optimization of Molybdenum Subnanoclusters on Graphene: A Consistent Approach toward Catalytic Applications” *Atomistic & Molecular-scale Modelling @ KCL 2023 (London, UK)*.
- **Wei Y**, “Computational materials discovery for lanthanide hydrides at high pressure for high temperature superconductivity” *2023 UK's HEC Materials Chemistry Consortium Conference (Daresbury UK)*.
- **Wei Y**, “DMFT method for the influence of f orbital on high temperature superconducting lanthanide hydride” *2022 Autumn School on Correlated Electrons (Jülich, Germany)*
- **Wei Y**, “Lanthanide hydrides exhibit high-temperature superconductivity at extreme pressure” *APS April Meeting 2022 (New York, USA)*. [Link](#)
- **Wei Y**, “The thrust characteristics of a novel transverse flux permanent magnet linear motor with the concentrated flux mover”. *2018 IEEE International Conference on Applied Superconductivity and Electromagnetic Devices (ASEMD), 2018 (Tianjin, China)*
- **Wei Y**, “Analysis of a novel flux switching transverse flux permanent magnet linear motor”. *2018 IEEE International Conference on Applied Superconductivity and Electromagnetic Devices (ASEMD), 2018 (Tianjin, China)*

Interests

- Beyond research, Yao is a keen traveller and travel writer. He has visited over 50 countries, authored a Chinese-language guide to public transport across the UK “30 Days · Public Transport Travel in the UK. Efficient, Affordable, and Easy” (ISBN 978-1-291-65704-3), and enjoys sharing his journeys and science with a wider audience through online writing.