Dr Yao Wei

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Research Profile: Computational condensed matter physicist specializing in strongly correlated electron theory (DMFT), high-pressure rare-earth hydride superconductivity, and ab initio global optimization of sub-nano metal cluster catalysts. Holder of an EU MSCA Fellowship under the Physics For Future Programme, with 15 peer-reviewed journal papers (8 first/co-first author), independent national supercomputing allocations, and cross-institutional research experience across the UK, Slovakia and Czech Republic.

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 absorbed species, Catalysis

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

MSc, Electronic engineering with management, King's College London, UK *09/2018 – 01/2020*

- Core Modules: Artificial Intelligence, Operations Research, Pattern Recognition

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Research & Independent Fellowship Experience

Czech Academy of Sciences, CZ

Marie Skłodowska -Curie Actions (MSCA) Fellow, Physics For Future Programme *2026 – now*

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**.
- Jointly explored many-body computational methods for correlated electron materials prior to commencing the Marie Skłodowska-Curie in Prague.

King's College London, UK

Visiting Senior Researcher Fellow (formally approved by the Faculty of Natural, Mathematical & Engineering Sciences) *08/2025 – now*

PhD Researcher *10/2020 – 08/2025*

- Supervised by: Lev Kantorovich, Jan Tomczak, Cedric Weber, Nicola Bonini.
- 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: Spearheaded the theoretical design of highly efficient catalytic surface matrices by anchoring and optimising metal atomic clusters. By determining the ideal atomic composition and cluster size for specific reactions, including carbon monoxide and water dissociation, this research provided direct computational guidance for experimental cluster deposition (Collaboration with Prof. Alessandro Baraldi at University of Trieste and Valera Veryazov at Lund University).

University of Cambridge, UK *2022 – 2024*

Visiting PhD Researcher

- 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: Extended the theoretical framework of dynamical mean field theory (DMFT) to incorporate rigorous phonon calculations. This methodological advancement overcame the inherent limitations of conventional density functional theory (DFT) when treating d and f electron systems, successfully enabling the precise evaluation of thermodynamic properties in strongly correlated materials.

Media Coverage / Press Releases

- Featured as a **Top Story on Elettra Sincrotrone Trieste official website**: "A new route to oxygen-rich nanomaterials". Highlighted our finding that Mo subnanoclusters on graphene/Ru(0001) take up oxygen well beyond the bulk limit, reaching Mo:O ratios of 1:4 and 1:5, through photon-driven fluxionality at cryogenic temperatures, where electrons generated by the X-rays drive structural rearrangements that thermal activation alone cannot (Sept 2026). Link
- Featured on **Thomas Young Centre official website**: "Correlation-driven phonon renormalization and the equation of state of γ-cerium". Highlighted a DFT+DMFT framework that couples cerium's correlated electrons to phonon calculations self-consistently, showing that electron-phonon feedback stiffens (rather than softens) certain vibrational modes and brings the predicted equation of state into close agreement with experiment (July 2026). Link
- *Correlation-driven phonon renormalization and the equation of state of γ-cerium*, Phys. Rev. B **114**, 055110 (2026), featured by Physical Review B as a **#PRBTopDownload** and highlighted on the journal's official X account (@PhysRevB) (20 July 2026). Link
- 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

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Publications

I. Book

[1] Wei Y, Kantorovich L, Weber C. Correlated Materials from First Principles: A Practical Introduction (provisional title). CRC Press (Taylor & Francis), under contract (signed November 2026; manuscript due 2028).

II. Journal Articles Selected Representative Publications

- Wei Y, Perco D, Santana-Bonilla A, et al., Photon-Driven Cluster Fluxionality: Breaking the Bulk Stoichiometry Ceiling in Sub-Nanometric Molybdenum Oxides. ACS Nano, 2026 20 (37), 25481–25491.
- Wei Y, Chen S, Plekhanov E, et al. Correlation-driven phonon renormalisation and the equation of state of γ-cerium [J]. Physical Review B, 2026, 114(5), 055110. (**First & Corresponding Author,**

#PRBTopDownload)

- 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. (**Co-first Author**)
- 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**)

III. Full List of Journal Publications

[15] Wei Y, Perco D, Santana-Bonilla A, et al., Photon-Driven Cluster Fluxionality: Breaking the Bulk Stoichiometry Ceiling in Sub-Nanometric Molybdenum Oxides. ACS Nano, 2026 20 (37), 25481–25491.

[14] Wei Y, Chen S, Plekhanov E, et al. Correlation-driven phonon renormalisation and the equation of state of γ-cerium [J]. Physical Review B, 2026, 114(5), 055110. (**First & Corresponding Author, #PRBTopDownload**)

[13] 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. (**Co-first Author**)

[12] 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.

[11] 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.

[10] 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.

[9] 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)**

[8] 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.

[7] 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.

[6] 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.

[5] 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.

[4] 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.

[3] 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.

[2] 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.

[1] Zhao W, Wei Y, Yang H Y, et al. Research on Topological Structure of Transverse Flux Switching Magnetic Chain Permanent Magnet Linear Motor[J]. Journal of Ludong University (Natural Science Edition), 2018, 34(1):14-19+37.

IV. Peer-Reviewed Conference Papers (Full Proceedings)

[2] Wei Y, Zhao M, Yang H, Deng G, Han F, Xu M, Zou J. Analysis of a novel flux switching transverse flux permanent magnet linear motor. In: 2018 IEEE International Conference on Applied Superconductivity and Electromagnetic Devices (ASEMD), 2018, pp. 1–2.

[1] Zhao M, Wei Y, Yang H, Feng N, Xu M, Hou D, Zou J. The Thrust Characteristics of a Novel Transverse Flux Permanent Magnet Linear Motor with the Concentrated Flux Mover. In: 2018 IEEE International Conference on Applied Superconductivity and Electromagnetic Devices (ASEMD), IEEE, 2018, pp. 1–2.

V. Conference Abstracts

[4] Wei Y, Santana-Bonilla A, Kantorovich L. A comprehensive exploration of structural and electronic properties of Molybdenum clusters. In: *Verhandlungen der Deutschen Physikalischen Gesellschaft*, **DPG Spring Meeting** Berlin 2024, Session O108.6. Link

[3] Wei Y, Chen S, Plekhanov E, Poncé S, Monserrat B, Weber C. Superconductivity of cerium hydride at high pressure from DFT+DFPT+DMFT. In: *Bulletin of the American Physical Society*, 2023 **APS March Meeting**, Vol.68, No.3, Abstract ID N20.00010. Link

[2] Wei Y, Weber C. Lanthanide hydrides exhibit high-temperature superconductivity at extreme pressure. In: *Bulletin of the American Physical Society*, 2022 **APS April Meeting**, Vol.67, No.6, Abstract ID K17.00049. Link

[1] Wei Y, Weber C. High-temperature superconductivity in the lanthanide hydrides at extreme pressures. In: *TYC Student Day 2022 Abstract Book*, Thomas Young Centre, Queen Mary University of London, London, UK. Link

VI. Manuscripts Under Revision & Review

[1] Wei Y, Hui Y, Li J, et al. Toward zero-carbon first-principles calculations with renewable-powered supercomputing [J]. Decarbon.

Conference Presentations and Posters

I. Oral Presentations

[8] Wei Y. Correlation-driven phonon renormalization and the equation of state of γ-cerium. Seminar, Department of Condensed Matter Theory, FZU – Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic, 20 October 2026.

[7] Wei Y. Carbon, oxygen and carbon monoxide adsorption on graphene-supported size-selected Mo clusters. Oral Presentation, **MMM Hub Conference & User Meeting** 2024, Battle of Britain Bunker, Uxbridge, UK, 29–31 October 2024.**(** Event webpage available Link**)**

[6] A comprehensive exploration of structural and electronic properties of Molybdenum clusters. Oral Talk, Session O108.6 Electronic Structure Theory II, **DPG Spring Meeting** Berlin 2024, Berlin, Germany, 22 March 2024, Room MA 043.

[5] Global Optimization of Molybdenum Subnanoclusters on Graphene: A Consistent Approach toward Catalytic Applications. Oral Presentation, 1st Atomistic & Molecular-scale Modelling @ KCL Workshop, King's College London, London, UK, 2023.(Event announcement available via LinkedIn official post Link)

[4] Computational materials discovery for lanthanide hydrides at high pressure for high temperature superconductivity. Oral Presentation, **MCC Conference** 2023 (UK HEC Materials Chemistry Consortium), Daresbury Laboratory, Daresbury, UK, 28 June 2023 (Official conference webpage available Link).

[3] Superconductivity of cerium hydride at high pressure from DFT+DFPT+DMFT. Oral Presentation, Session N20: Matter at Extreme Conditions: Simulation and Novel Methods, **APS March Meeting**, Las Vegas, NV, USA, 08 March 2023.

[2] Wei Y. High-temperature superconductivity in the lanthanide hydrides at extreme pressures. Oral Presentation, **TYC Student Day** 2022, Queen Mary University of London, London, UK, 10 May 2022.(Event webpage available Link)

[1] The Thrust Characteristics of a Novel Transverse Flux Permanent Magnet Linear Motor with the Concentrated Flux Mover. Oral Presentation, 2018 **IEEE International Conference on Applied Superconductivity and Electromagnetic Devices (ASEMD)**, Tianjin, China, 18 April 2018.

II. Poster Presentations

[3] Wei Y. Rational Design of Molybdenum Transition-Metal subnanoclusters catalysts with Particle Swarm Optimization. Poster Presentation, TYC Postgraduate Student Day 2024, Royal School of Mines, Imperial College London, London, UK, 22 May 2024. (Event webpage Link)

[2] Wei Y. Lanthanide hydrides exhibit high-temperature superconductivity at extreme pressure. Poster Presentation, Session K17 Poster Session II, APS April Meeting 2022, New York, USA, 10 April 2022, 9th Floor Terrace.

[1] Wei Y. DMFT method for the influence of f orbital on high temperature superconducting lanthanide hydride. Poster Presentation, 2022 Autumn School on Correlated Electrons: Dynamical Mean-Field Theory of Correlated Electrons, Forschungszentrum Jülich, Germany, 4–7 October 2022. (Official conference webpage available Link)

Grants, HPC Allocations & Competitive Awards

- **Marie Skłodowska-Curie Actions (MSCA) Fellow**, Physics for Future (P4F) Programme. 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, but unfunded due to agency budget constraints)** by independent evaluators; ranked top. Excellence recognized in ab initio superconductivity, open-source tools, and international collaboration (submitted Nov 2025; evaluated Apr 2026).
- **IT4I Czech National Supercomputing Allocations** (Independent PI, 2026–)
  2026 Oct-: 4M CPUh
- **Archer2 UK National Supercomputing Allocations** (Independent PI, 2023–2026)
  2026 Jan–Jun: 6M CPUh (~£18,000 equivalent resource funding)
  2025: 22M CPUh (~£65,000 equivalent resource funding)
  2024: 24M CPUh (~£74,000 equivalent resource funding)
  2023: 2M CPUh (~£8,190 equivalent resource funding)
- **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.** (Full tuition fee + monthly living allowance) (2020-2025)
- **American Physical Society (APS) Distinguished Student Program (DS)** (Prize of $500) (2023)
- King's Student Opportunity Fund (Prize of £500) (2023-2024)
- King's Student Opportunity Fund (Prize of £500) (2022-2023)
- King's London Experience Award (2019)

Academic Services & Editorial Roles

Peer Review

Referee, Advanced Quantum Technologies (Wiley), 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.

King's College London, UK

Graduate Teaching Associate *10/2020 – 08/2025*

- 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).

Materials and Molecular Modelling Hub & Thomas Young Centre, UK

Activities & Conferences Co-organizer *2023 – 2024*

- 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.

Professional Memberships

- Marie Curie Alumni Association (MCAA), Member *2026 – present*
- American Chemical Society (ACS), Member *2025 – 2027*
- Royal Meteorological Society (RMetS), Member *2023 – 2024*
- American Physical Society (APS), Member *2022 – 2023*
- Institution of Engineering and Technology (IET), Member *2018 – 2019*

Teaching & Mentorship Experience

King's College London, UK

Independent Student Mentor *08/2025-now*
The mentor of Success for Black Students Program *08/2024—08/2025*
Rep of Staff Student Liaison Committee *09/2023—09/2024*

- Independently supervise undergraduate students from King's College London and Imperial College London on first-principles material simulation projects, including DFT calculation workflow training, result analysis and manuscript drafting guidance.
- Provide regular one-on-one research supervision to internal Ph. D. candidates, supporting their work on correlated electron systems and high-pressure superconductivity; assist with project design, computational troubleshooting and paper revision.
- 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.
- Collaborated with faculty to ensure course alignment with departmental and university standards.

London School of Economics and Political Science (LSE), UK

Tutor, Confucius Institute at LSE *06/2022—09/2022*

- Delivered Chinese language classes to international students, promoted cross-cultural communication and cultural outreach activities.

Technical Computational Skills

- **Electronic Structure & Many-Body Methods:** VASP, WIEN2k, CP2K, Quantum ESPRESSO, EDMFTF (DMFT), CASTEP, PHONOPY, TDEP.
- **Programming & Scripting:** Python (NumPy, SciPy, ASE, Matplotlib), Bash
- **Machine Learning & Data-Driven Modelling:** Dimensionality reduction (PCA) and neural-network surrogate models for interpolating first-principles observables; global optimisation with particle swarm methods over ab initio energy landscapes; scikit-learn, PyTorch.

Outreach & Additional Information

- Keen traveller and travel writer; visited 60+ countries and regions and authored a Chinese-language UK public-transport guide, "30 Days · Public Transport Travel in the UK" (ISBN 978-1-291-65704-3) Link. Also active in public science and cultural outreach, including work as an independent tour guide across the UK.