Lei Ge

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CURRENT APPOINTMENTS

Imperial College London, London, UK — Aug 2023 – Expected Sep 2026
PhD Candidate in Design Engineering

- Current research focuses on LLMs for materials science, interpretable AI, and agentic systems.

Polaron, London, UK — Jun 2025 – Present
Part-time LLM Machine Learning Engineer

- Led the development of an LLM agent platform, bridging research and real-world deployment.

RESEARCH INTERESTS

Large language models | AI for materials science | LLM agents | interpretable AI

EDUCATION

Imperial College London, London, UK — 2023 – Expected 2026
PhD in Design Engineering
Supervisor: Dr. Samuel J. Cooper

- Research focus: LLMs for science, LLM agents, and AI interpretability
- Lee Family Scholarship (full scholarship awarded to 1–2 top Chinese candidates annually)

Donghua University, Shanghai, China — 2020 – 2023
MSc in Fashion Design and Engineering

- GPA: 91/100; thesis grade: 92.6/100
- Thesis: *A Computer Vision-Based Graphic Coding Technique for Garment Development*
- Awards: Outstanding Master's Thesis (top 2%), China National Scholarship (top 0.2%), Outstanding Student Award (top 0.2%), Shanghai Outstanding Graduate (top 5%)

Donghua University, Shanghai, China — 2016 – 2020
BEng in Fashion Design and Engineering

- GPA: 90.3/100
- Awards: China National Scholarship (twice; top 0.2%), Outstanding Student Award (twice; top 0.2%), Donghua Outstanding Graduate Award (top 15%)

Istituto Marangoni — 2018 – 2019
Exchange Student in Fashion Design

- Developed seasonal fashion collections and portfolio work, covering concept development, pattern-making, and garment construction.

PUBLICATIONS

[P1] **Lei Ge** and Samuel J. Cooper. *Elicitation Matters: How Prompts and Query Protocols Shape LLM Surrogates under Sparse Observations*. arXiv:2605.04764, 2026.

[P2] **Lei Ge**, Ferran B. Planella, Stephen G. Baird, and Samuel J. Cooper. *From Prompt to Protocol: Fast Charging Batteries with Large Language Models*. arXiv:2601.09626, 2026.

[P3] **Lei Ge** and Samuel J. Cooper. *Do Llamas Understand the Periodic Table? Digital Discovery*, 4(12):3455–3465, 2025.

[P4] **Lei Ge**, Ronan Docherty, and Samuel J. Cooper. *Materials Science in the Era of Large Language Models: A Perspective*. *Digital Discovery*, 3(7):1257–1272, 2024.

[P5] **Lei Ge** and Xiaohui Li. *A Vision-Based Approach to Mapping Flexible Objects for Garment Development*. *Textile Research Journal*, 93(15–16):3381–3395, 2023.

[P6] **Lei Ge** and Xiaohui Li. *A New Approach to 3D Pattern-Making for the Apparel Industry: Graphic Coding-Based Localization*. *Computers in Industry*, 136:103587, 2022.

[P7] **Lei Ge** and Xiaohui Li. *Review of Digital Pattern-Making Technology in Garment Production*. *Journal of Textile Research*, 43(4):203–209, 2022.

[P8] **Lei Ge** and Xiaohui Li. *A Pattern-Making Approach to Improving Zero-Waste Fashion Design*.

Fashion Practice, 13(3):443–463, 2021.

SELECTED PRESENTATIONS

[T1] **Lei Ge**. *From Trust to Action: Large Language Models for Scientific Discovery and Decision Support*. AI in Metallurgy (AIMET), Mechelen, Belgium, 2026 (Keynote)

[T2] **Lei Ge**. *Do Llamas See the Periodic Table in 3D? Geometry and Layerwise Representations*. NeurIPS 2025 AI for Science Workshop, San Diego, USA, 2025. (Spotlight)

[T3] **Lei Ge**. *From Prompt to Protocol: Fast Charging Batteries with Large Language Models*. AI4AM 2026, Madrid, Spain, 2026. (Oral)

[T4] **Lei Ge**. *Unveiling 3D Geometries in LLMs: The Representation and Recall of Periodic Elements*. AI4AM 2025, San Sebastian, Spain, 2025. (Oral)

[T5] **Lei Ge**. *Large Language Models in Materials Science*. L2M3: Large Language Models for Materials, Molecules and Beyond, EPFL, Switzerland, 2024. (Oral)

[T6] **Lei Ge**. *LLMs Know Chemistry: Representation of the Periodic Table in Large Language Models*. Oxford Modelling Symposium, Oxford, UK, 2025. (Poster)

[T7] **Lei Ge**. *Battery GPT? Materials Science in the Era of Large Language Models*. Oxford Modelling Symposium, Oxford, UK, 2024. (Poster)

[T8] **Lei Ge**. *Do Llamas Understand Chemistry?* AI for Materials Summer School, Karlsruhe, Germany, 2025. (Poster)

ACADEMIC SERVICE

Co-organizer & Speaker, *Deep Matters: Foundations* [website] 2025
Google Cloud Startup Hub, London, UK

- Co-organized an interdisciplinary conference on foundation models for materials science with approximately 100 attendees.
- Served as one of the organizers across programme development, speaker coordination, sponsorship, logistics, and event delivery.
- Secured sponsorship from Google and Polaron and coordinated invited speakers from NVIDIA, UCL, Orbital, CuspAI, and Imperial College London.

Invited Lecturer, iCircular^3 Marie Curie Doctoral Network 2025

- Delivered the lecture *How LLMs Work? From Transformer to Reasoning* for doctoral researchers in the MSCA-DN programme.

RESEARCH EXPERIENCE

LLM Surrogate Belief under Sparse Observations **Imperial** | 2026
Study how large language models behave as surrogate models under sparse observations in low-data optimization. This work shows that prompt design and query protocol are not merely interface choices, but core components of surrogate specification that materially affect uncertainty, belief updating, and downstream decision-making. The project provides a practical framework for evaluating and improving the reliability of LLM-based surrogates in scientific optimization and AI for science workflows.
Associated output: [P1].

LLM-Guided Optimization for Battery Charging Protocols **Imperial** | 2025
Develop LLM agents for battery fast-charging protocol optimization. This work shows that LLMs can expand protocol search beyond fixed human-designed parameterizations, incorporate natural-language safety constraints, and enable effective optimization in expensive, slow-feedback scientific settings.
Associated outputs: [P2].

Knowledge Representation in Large Language Models **Imperial** | 2024 – 2025
Investigate how large language models encode structured scientific knowledge. This work observes a 3D spiral structure in the hidden states of LLMs that aligns with the conceptual structure of the periodic table, suggesting that LLMs can reflect the geometric organization of scientific concepts learned from text.
Associated outputs: [P3], [T2], [T4], [T6], [T8].

Automation and Knowledge Extraction for Scientific Data **Imperial** | 2023 – 2024
Build automated AI systems for extracting, structuring, and operationalizing scientific knowledge from literature and imaging workflows. Developed *MicroGPT* for 3D microstructure analysis and pipelines

for extracting and labeling datasets from academic papers.
Associated outputs: [P4], [T5], [T7].

Vision-Based 3D Garment Mapping and Pattern Development **DHU** | 2020 – 2022
Develope computer-vision-based methods for mapping flexible garment surfaces and translating 3D shape information into structured representations for garment development. This work connected coded visual localization, geometric reconstruction, and digital pattern development for apparel applications.
Associated outputs: [P5], [P7].

AI-Enabled Personalized Fashion Design Systems **DHU** | 2022 – 2023
Develope AI-enabled approaches for personalized fashion design and garment customization, with a focus on translating individual body features and user-specific design needs into structured pattern-making and apparel development workflows. This work explored how computational design methods can support intelligent made-to-measure garment creation and personalized clothing production.
Associated outputs: [P6].

Zero Waste Fashion Pattern Design **DHU** | 2019 – 2022
Explore computational approaches to garment pattern-making with an emphasis on sustainability and manufacturability. This research investigated how structured pattern design methods can support zero-waste fashion design while preserving fit, function, and design intent.
Associated outputs: [P8].

INDUSTRY EXPERIENCE

Polaron, London, United Kingdom June 2025 – Present
LLM Machine Learning Engineer (Part-time)

- Built a production-oriented LLM orchestration service with FastAPI, LangGraph, and AWS Bedrock, enabling natural-language control over internal workflows via structured tool calling.
- Designed the agent runtime for multi-turn dialogue, streaming, tool execution loops, interruption/resume flows, and failure recovery guardrails.
- Implemented typed tool contracts, approval-aware workflow actions, sandboxed code execution, artifact handling, and retrieval over product documentation.
- Added Redis/Postgres/S3-backed persistence, checkpointing, audit logging, redacted tracing, readiness checks, and benchmark/test coverage.

Target, Shanghai, China Dec 2022 – Mar 2023
Management Trainee (Full-time)

- Completed rotational training across Packaging, Color, Technical Design, Quality Assurance, and Sustainability, gaining comprehensive insight into product development.
- Contributed to a sustainability initiative transforming recycled plastic bottles into home textiles.

Chenfeng Group, Changzhou–Wuxi–Suzhou, China Jun 2021 – Jul 2021
Program Intern

- Rotated across the fashion design department, intelligent sewing workshop, and textile inspection department to gain cross-functional exposure in apparel manufacturing.

H&M, Shanghai, China Sep 2019 – Dec 2019
Merchandising Assistant Intern

- Supported merchandisers in workflow execution, created product forms and color charts, and facilitated communication with suppliers.

Target, Shanghai, China Jul 2019 – Aug 2019
Product Design and Development Intern

- Designed zero-waste children's wear for "LTO Back to School," integrating sustainability across materials, manufacturing, and retail.
- Supported Target Own Brand development through market research, supplier visits, and BPFE certification feedback.

REVIEWING EXPERIENCE

Journal Reviewer
Communications Materials; *npj Computational Materials*; *Digital Discovery*; *RSC Advances*