Lei Zhang

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Summary

Postdoctoral researcher applying NLP and machine learning for data-driven electrocatalyst discovery. Creator of MatNexus, an open-source framework for automated literature collection, text mining, and embedding-based property prediction. Current work integrates NLP, multi-modal learning, and optimisation with experimental validation.

Education

PhD in Materials Science <div align="right">2022–2025</div>
Ruhr University Bochum (ICAMS), Germany
Thesis: *Accelerating Materials Discovery through Text Mining and Machine Learning: A Data-Driven Approach*
Supervisor: Prof. Markus Stricker (<u>link</u>)

Master's Degree in Materials Science <div align="right">2019–2022</div>
NanChang Hangkong University, China
Thesis: *Electrocatalyst Design and Preparation: A Laboratory-Based Approach*

Bachelor's Degree in Welding Technology <div align="right">2013–2017</div>
NanChang Hangkong University, China

Research Experience

Postdoctoral Researcher, Ruhr University Bochum (ICAMS) <div align="right">2025–Present</div>

- Extending MatNexus with advanced NLP, multi-modal learning, and optimisation for materials discovery.
- Leading collaborations with experimental groups (incl. Prof. Alfred Ludwig's team: <u>link</u>) to prioritise candidate compositions and validate predictions.
- Contributing to CRC 1625 (<u>link</u>), DIMENSION (<u>link</u>), and COST CA22154 (<u>link</u>).

PhD Researcher, Ruhr University Bochum (ICAMS) <div align="right">2022–2025</div>

- Developed MatNexus: automated literature mining + word-embedding pipelines for materials discovery.
- Built Python workflows for data curation, NLP, model training/evaluation; supported composition–property prediction.
- Collaborated with experimental partners for synthesis guidance and validation.

Master's Researcher, NanChang Hangkong University <div align="right">2019–2022</div>

- Experimental electrocatalyst development (molten-salt synthesis, scale-up, electrochemical evaluation)

Publications

PhD / Current Research

Peer-reviewed

1. **Zhang, L.** and Stricker, M. *MatNexus: A comprehensive text mining and analysis suite for materials discovery. SoftwareX* 26 (2024). DOI: 10.1016/j.softx.2024.101654
2. **Zhang, L.**, Banko, L., Schuhmann, W., Ludwig, A., Stricker, M. *Composition-property extrapolation for compositionally complex solid solutions based on word embeddings. Digital Discovery* (2025). DOI: 10.1039/D5DD00169B
3. **Zhang, L.** and Stricker, M. *Iterative Corpus Refinement for Materials Property Prediction Based on Scientific Texts.* ECML PKDD (2025). DOI: 10.1007/978-3-032-06118-8_6
4. Stricker, M., Banko, L., Sarazin, N., Siemer, N., Janssen, J., **Zhang, L.**, Neugebauer, J., Ludwig, A. *Computationally accelerated experimental materials characterization. Nature Communications* (2026). DOI: 10.1038/s41524-025-01919-5.

Preprints

1. **Zhang, L.** and Stricker, M. *Electrocatalyst discovery through text mining and multi-objective optimization.* arXiv (2025). arXiv:2502.20860

Master's Research

Peer-reviewed

1. Hu, Z., Chen, Z., Huang, J., Yan, M., Zhang, M., **Zhang, L.**, Li, X., Feng, Z. *Graphene-based SiC nanowires with nanosheets. CrystEngComm* 22(24) (2020) 4074–4078. DOI: 10.1039/d0ce00297f
2. Hu, Z., **Zhang, L.**, Huang, J., et al. *Self-supported Ni-doped Mo_2C nanoflowers on CFP for HER. Nanoscale* 13(17) (2021) 8264–8274. DOI: 10.1039/d1nr00169h
3. Yan, M., Xiong, Q., Huang, J., **Zhang, L.**, et al. *Molten salt synthesis of TiC using carbon templates. Ceramics International* 47(12) (2021) 17589–17596. DOI: 10.1016/j.ceramint.2021.03.077
4. **Zhang, L.**, Huang, J., Hu, Z., et al. *Ni-doped Mo_2C@CFP electrode via molten salt for HER. Rare Metal Materials and Engineering* 51(4) (2022) 1341–1347.
5. **Zhang, L.**, Huang, J., Li, X., et al. *$Ni(NO_3)_2$-induced WC coating on CFP for HER via molten salt. Electrochimica Acta* 422 (2022) 140553. DOI: 10.1016/j.electacta.2022.140553
6. **Zhang, L.**, Hu, Z., Huang, J., et al. *Experimental and DFT studies of Ni-doped Mo_2C on CFP for HER. Journal of Advanced Ceramics* 11(8) (2022) 1294–1306. DOI: 10.1007/s40145-022-0610-6
7. Luo, Z., **Zhang, L.**, Huang, J., et al. *Ni-doped WC/Mo_2C on CFP via molten salt for HER. Ceramics International* 49(11A) (2023) 17993–17999. DOI: 10.1016/j.ceramint.2023.02.073
8. Ding, T., **Zhang, L.**, Huang, J., et al. *P-Ni co-doped Mo_2C embedded in carbon-fiber paper for alkaline HER. Diamond and Related Materials* 143 (2024) 110942. DOI: 10.1016/j.diamond.2024.110942

Patents

- CN113072069A; CN113073351A; CN110368969A.

Conference Presentations

- 2025 – AIMSE2025 (Bochum, Germany): "Literature-Based Prediction of High-Performance Electrocatalysts."
- 2025 – ECML PKDD (Porto, Portugal): "Iterative Corpus Refinement for Materials Property Prediction Based on Scientific Texts."
- 2024 – MLM4MS (Ljubljana, Slovenia): "Prediction of quaternary systems based on word embeddings."
- 2024 – MMM11 (Prague, Czech Republic): "Vector analysis for improved prediction of quaternary material systems."
- 2024 – Early Career Researchers Day, RUB (Bochum, Germany): "MatNexus: text mining suite for materials discovery."
- 2023 – FEMS EUROMAT (Frankfurt, Germany): "From text data to word embeddings in Materials Science."
- 2023 – GC-MAC Summer School (KIT Karlsruhe, Germany): "MatNexus: systematic text extraction in materials science."
- 2022 – WE-Heraeus-Seminar (Bad Honnef, Germany): "From text data to word embeddings in Materials Science."

Fellowships, Awards, and Grants

- Research Fellowship, RUB — 2025
- Doctorate with Distinction — 2025
- CSC Scholarship — 2022–2025
- First Place, Science Slam (RUB) — 2024
- Excellent Graduate Student — 2022
- Jiangxi Gov. Scholarship — 2021
- First Class Postgraduate Scholarship — 2019–2022
- Microstructure Photography (1st Prize) — 2020
- Postgraduate Forum (1st Prize) — 2020
- National Scholarship — 2017
- NCHU Scholarship — 2013–2017

Teaching Experience

- Mentor, course project (2024): *Comparative Analysis of Descriptors in Electrocatalysis.*
- Supervisor, student assistant (2024): data collection/analysis and text-mining workflows for materials discovery.