

# Lei Zhang

Postdoctoral Researcher, Ruhr University Bochum (ICAMS)

**Website:** leizhanglab.com

**Email:** Lei.Zhang-w2i@ruhr-uni-bochum.de

ORCID: [link](#) Google Scholar: [link](#) ResearchGate: [link](#)

## 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

<b>PhD in Materials Science</b>	2022–2025
Ruhr University Bochum (ICAMS), Germany	
Thesis: <i>Accelerating Materials Discovery through Text Mining and Machine Learning: A Data-Driven Approach</i>	
Supervisor: Prof. Markus Stricker ( <a href="#">link</a> )	
<b>Master's Degree in Materials Science</b>	2019–2022
NanChang Hangkong University, China	
Thesis: <i>Electrocatalyst Design and Preparation: A Laboratory-Based Approach</i>	
<b>Bachelor's Degree in Welding Technology</b>	2013–2017
NanChang Hangkong University, China	

### Research Experience

**Postdoctoral Researcher**, Ruhr University Bochum (ICAMS) 2025–Present

- Extending MATNEXUS with advanced NLP, multi-modal learning, and optimisation for materials discovery.
- Leading collaborations with experimental groups (incl. Prof. Alfred Ludwig’s team: [link](#)) to prioritise candidate compositions and validate predictions.
- Contributing to CRC 1625 ([link](#)), DIMENSION ([link](#)), and COST CA22154 ([link](#)).

**PhD Researcher**, Ruhr University Bochum (ICAMS) 2022–2025

- 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 2019–2022

- 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<sub>2</sub>C 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<sub>2</sub>C@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<sub>3</sub>)<sub>2</sub>-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<sub>2</sub>C 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<sub>2</sub>C 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<sub>2</sub>C 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	• First Class Postgraduate Scholarship	2019–2022
• Doctorate with Distinction	2025	• Microstructure Photography (1st Prize)	2020
• CSC Scholarship	2022–2025	• Postgraduate Forum (1st Prize)	2020
• First Place, Science Slam (RUB)	2024	• National Scholarship	2017
• Excellent Graduate Student	2022	• NCHU Scholarship	2013–2017
• Jiangxi Gov. Scholarship	2021		

#### 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.