

Mohd Zaki

Postdoctoral Researcher,
Hopkins Extreme Materials Institute,
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Professional Experience

- **Postdoctoral Researcher, Johns Hopkins University** — Feb, 2025 - ongoing
  Topic: Discovering materials for extreme environments through Agentic AI
  PI: Prof. Michael D. Shields

Education

- **Ph.D., Structural Engineering – (CGPA 9.214/10)** — 2019 – 2025
- Dept. of Civil Engineering, Indian Institute of Technology Delhi
- Thesis title: Machine learning and natural language processing for construction materials
- Supervisors: Prof. N. M. Anoop Krishnan and Prof. Jayadeva

B.Tech., Civil Engineering – (CGPA: 8.57/10) — 2013 – 2017
- Dept. of Civil Engineering, Motilal Nehru National Institute of Technology Allahabad, India

Class XII (CBSE) – 479/500 (95.8%) — 2013
- S.S. Children Senior Secondary School, Moradabad, India

Class X (CBSE) – CGPA 10.0/10.0 — 2011
- S.S. Children Senior Secondary School, Moradabad, India

Scholastic Awards and Achievements

- USACM Travel and Registration grant for WCCM-ECCOMAS 2026 — 2026
- AI4MAT-ICLR 2026 Travel Grant — 2026
- Best poster award in AI for materials science at inaugural Hopkins Extreme Materials Institute conference — 2024
- 3-Minute Thesis presentation award, Open House, IIT Delhi — 2024
- Travel, registration, and accommodation grant by 5th Indian Symposium on Machine learning, BITS Pilani, Goa — 2024
- Travel, registration, and accommodation grant by 4th Indian Symposium on Machine learning, IIT Bombay, Mumbai — 2023
- Travel grant by Industrial Research and Development Unit, IIT Delhi for presenting at 2023 MRS Fall Conference, Boston, USA — 2023
- ACL D&I grant for attending 61st ACL Conference, Toronto, Canada — 2023
- SERB International Travel Support Grant for presenting at 2023 MRS Spring Conference, San Francisco, USA — 2023
- Prime Minister's Research Fellowship (PMRF) — 2020-2024
- Meritorious student scholarship award in Civil Engineering Department, Motilal Nehru National Institute of Technology, Allahabad — 2013-2017
- Summer Research Internship, Indian Institute of Technology Mandi — 2015
- DST INSPIRE Internship — 2011

Technical Skills

- Programming languages: Python, C, FORTRAN
- Tools and Utilities: Cursor, MATLAB, OpenSees, AutoCAD, STAAD Pro, Revit Architecture, Robotic platforms: Arduino, Raspberry Pi, NVIDIA Jetson Nano

Teaching Experience

- CVP441: Structural Design and Detailing (100 students, UG, designing structures in STAAD Pro. and drawing in AutoCAD) — 2020 – 2023, 2021 – 2022
- CVL757: Finite Element Methods in Structural Engineering (30 students, UG, Master, and PhD, introduced Python programming based assignments for finite element analysis) — 2020 – 2021
- MLL703: Mathematical and Computational Methods in Materials (30 students, Masters and PhD, numerical differentiation, integration methods, MATLAB and Python based programming assignments) — 2020 – 2021
- ELL409(UG) and ELL784(PG): Introduction to Machine Learning (60 students, logistic support, and hands-on session for using high performance computing cluster at IIT Delhi)

Conferences

1. 17th World Congress on Computational Mechanics & 10th European Congress on Computational Methods in Applied Sciences and Engineering, Munich, Germany, July 19th-24th, 2026
    a. Uncertainty Quantification of Foundation Models for Scientific Machine Learning
2. AI4MAT workshop at ICLR-2026, Rio de Janeiro, Brazil, April 26th, 2026.
    a. Materials Research Agent
3. SIAM Conference on Uncertainty Quantification (2026), Minneapolis, Minnesota, March 22-25, 2026
    a. Uncertainty quantification across the lifecycle of foundation models for scientific machine learning
4. Inaugural High Performance Computing Symposium, Johns Hopkins University., April 2, 2025.
    a. Automated information extraction for ceramic materials
5. 10th International Conference on CONcrete under SEvere Conditions Environment & Loading, September 25th - 27th , 2024
    a. AI Driven Information Extraction From Construction Materials Literature
6. Engineering Mechanics Institute Conference 2024 (EMI-2024), May 28th – 31st, 2024, Chicago, Illinois, USA
    a. CEMCAT: Cementitious materials catalogue with their compositions, properties, synthesis and characterization methods, and applications
7. Glass and Optical Materials Division Meeting (GOMD 2024), May 19th – 24th, 2024, Las Vegas, Nevada, USA
    a. Extracting materials tetrahedron of inorganic glasses using natural language processing
8. 2023 Materials Research Society Meeting & Exhibit, November 26th – December 1st , 2023, Boston, Massachusetts, USA
    a. Large language models for materials science education and research
    b. Information extraction from materials science research papers
9. 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), pages 13465–13483, Toronto, Canada. Association for Computational Linguistics, 2023
    a. DiSCoMaT: Distantly Supervised Composition Extraction from Tables in Materials Science Articles
10. Glass and Optical Materials Division Meeting (GOMD2023), June 4 - 8, 2023, New Orleans, Louisiana, USA (Oral)
    a. Automated extraction of glass compositions and properties from research literature
11. Engineering Mechanics Institute Conference 2023 (EMI-2023), June 6 - 10, 2023, Atlanta, Georgia, USA (Oral)
    a. Investigating large language models' understanding of mechanics
12. 2023 Materials Research Society Meeting & Exhibit, April 10 - 14, 2023, San Francisco, California, USA (Oral)
    a. Extracting materials Compositions from research papers using natural language processing
13. 26th International Congress on Glass, 2022 (Oral presentations, Online)
    a. Predicting Vickers Hardness of Glasses as a function of processing parameters.
    b. Predicting Optical properties of Glasses as a function of testing parameters.
14. Şişecam 37th International Glass Conference, Istanbul, Turkey, 2022
    a. Machine Learning Based Predictions and Explanations of Glasses Properties as a Function of Composition, Testing, and Processing Parameters (Poster)
15. Pacific Rim Conference on Ceramic and Glass Technology including Glass and Optical Materials Division Meeting (GOMD2022) (Oral presentations, Online):
    a. Predicting electrical properties of Glasses as a function of composition and wavelengths
16. Pacific Rim Conference on Ceramic and Glass Technology including Glass and Optical Materials Division Meeting (GOMD2021) (Oral presentations, Online):
    a. Predicting Normal and Anomalous Glasses Directly from the Indent Images using Machine Learning

b. Extracting the Synthesis and Processing Protocols from Materials Science Literature for Improved Property Prediction
c. Understanding the optical properties of glasses using interpretable machine learning

17. Material Science & Technology 2021 (MS&T21) (Oral presentations, Online):
    a. Elucidating Compositional Governance of Optical Properties Oxide Glasses Using Interpretable Machine Learning
    b. Predicting Glass Behavior from Optical Microscopy Images Using Interpretable Machine Learning

Reviewing Experience

Reviewed more than 40 research papers in reputed journals like Computational Materials, Journal of Physics: Materials, Journal of Non-Crystalline Solids, Journal of American Ceramics Society, Digital Discovery, and conference venues (ACL ARR, Computational Linguistic conferences, and AI4MAT and AI4Science NeurIPS Workshops) — 2021 – Present

Publications

1. **Zaki M**, Ahlawat D, Mishra V, Singh S, Bihani V, Grover H, Mishra B, Miret S, Mausam M, Krishnan NMA, LLaMat: A family of large language models for materials research with insights into model adaptability in continued pre-training. Nature Machine Intelligence. 2026 Feb 27;1-14
2. Mandal I, Soni J, **Zaki M**, Smedskjaer MM, Wondraczek K, Wondraczek L, Gosvami NN, Krishnan NMA. Evaluating large language model agents for automation of atomic force microscopy. Nature Communications. 2025 Oct 14;16(1):9104.
3. Hira K, **Zaki M**, Krishnan NMA, Mausam M. MatSKRAFT: A framework for large-scale materials knowledge extraction from scientific tables. arXiv preprint arXiv:2509.10448. 2025 Sep 12.
4. **Zaki M**, Bharadwaj K, Goyal R, Jayadeva J, Krishnan NMA. Artificial intelligence for information extraction from cement literature. In Binding Materials for Sustainable Construction 2025 Jan 1 (pp. 819-832). Woodhead Publishing.
5. Mishra V, Singh S, **Zaki M**, Grover HS, Miret S, Mausam, Krishnan NMA. LLaMaT: Large Language Model for Materials Science. AI4MAT Workshop, BOKU Vienna (accepted, July, 2024)
6. **Zaki M**, Jayadeva J, Mausam M, Anoop Krishnan NM. MaScQA: Investigating Materials Science Knowledge of Large Language Models. Digital Discovery. 2024. https://doi.org/10.1039/D3DD00188A
7. **Zaki M**, Jan A, Krishnan NMA, Mauro JC. Glassomics: An omics approach toward understanding glasses through modeling, simulations, and artificial intelligence. MRS Bulletin. 2023. https://doi.org/10.1557/s43577-023-00560-1
8. Hira K, **Zaki M**, Sheth D, Krishnan N, others. Reconstructing materials tetrahedron: Challenges in materials information extraction. Digital Discovery special issue on AI4MAT NeurIPS-2023 (accepted, 2024)
9. Mannan S, **Zaki M**, Bishnoi S, et al. Glass hardness: Predicting composition and load effects via symbolic reasoning-informed machine learning. Acta Materialia. 2023;255:119046. https://doi.org/10.1016/j.actamat.2023.119046
10. **Zaki M**, Sharma S, Gurjar SK, Goyal R, Krishnan NA, others. Cementron: Machine learning the alite and belite phases in cement clinker from optical images. Construction and Building Materials. 2023;397:132425.
11. Gupta T, **Zaki M**, Khatsuriya D, Hira K, Krishnan NMA, Mausam M. DiSCoMaT: Distantly supervised composition extraction from tables in materials science articles. Proceedings of the 61st annual meeting of the association for computational linguistics (volume 1: Long papers). Toronto, Canada: Association for Computational Linguistics; 2023:13465–13483. https://doi.org/10.18653/v1/2023.acl-long.753
12. Singla S, Mannan S, **Zaki M**, Krishnan NA. Accelerated design of chalcogenide glasses through interpretable machine learning for composition–property relationships. Journal of Physics: Materials. 2023;6(2):024003.

13. **Zaki M**, Kasimuthumaniyan S, Sahoo S, Jayadeva, Gosvami NN, Krishnan NMA. Interpretable Machine Learning Approach for Identifying the Tip Sharpness in Atomic Force Microscopy. Scripta Materialia. 2022;221:114965. https://doi.org/10.1016/j.scriptamat.2022.114965
14. Bhattoo R, Bishnoi S, **Zaki M**, Krishnan NMA. Understanding the compositional control on electrical, mechanical, optical, and physical properties of inorganic glasses with interpretable machine learning. Acta Materialia. 2023;242:118439. https://doi.org/10.1016/j.actamat.2022.118439
15. **Zaki M**, Namireddy SR, Pittie T, et al. Natural language processing-guided meta-analysis and structure factor database extraction from glass literature. Journal of Non-Crystalline Solids: X. 2022;15:100103. https://doi.org/10.1016/j.nocx.2022.100103
16. Gupta T, **Zaki M**, Krishnan NMA, Mausam M. MatSciBERT: A materials domain language model for text mining and information extraction. npj Computational Materials. 2022;8(1):102. https://doi.org/10.1038/s41524-022-00784-w
17. **Zaki M**, Venugopal V, Bhattoo R, et al. Interpreting the optical properties of oxide glasses with machine learning and Shapely additive explanations. Journal of the american ceramic society. 2022;105(6):4046–4057.
18. Lyngdoh GA, Li H, **Zaki M**, Krishnan NMA, Das S. Elucidating the constitutive relationship of calcium–silicate–hydrate gel using high throughput reactive molecular simulations and machine learning. Sci Rep. 2020;10(1):21336. https://doi.org/10.1038/s41598-020-78368-1
19. Ravinder, Venugopal V, Bishnoi S, … **Zaki M,** … et al. Artificial intelligence and machine learning in glass science and technology: 21 challenges for the 21st century. Int J Appl Glass Sci. 2021;12(3):277–292. https://doi.org/10.1111/ijag.15881
20. Venugopal V, Sahoo S, **Zaki M**, Agarwal M, Gosvami NN, Krishnan NMA. Looking through glass: Knowledge discovery from materials science literature using natural language processing. Patterns. 2021;2(7):100290. https://doi.org/10.1016/j.patter.2021.100290
21. Sharma V, **Zaki M**, Jha KN, Krishnan NMA. Machine learning-aided cost prediction and optimization in construction operations. Engineering, Construction and Architectural Management. 2021. https://doi.org/10.1108/ECAM-10-2020-0778
22. **Zaki M**, Jayadeva, Krishnan NMA. Extracting processing and testing parameters from materials science literature for improved property prediction of glasses. Chemical Engineering and Processing - Process Intensification. 2022;180:108607. https://doi.org/10.1016/j.cep.2021.108607
23. Lyngdoh GA, **Zaki M**, Krishnan NMA, Das S. Prediction of concrete strengths enabled by missing data imputation and interpretable machine learning. Cement and Concrete Composites. 2022;128:104414. https://doi.org/10.1016/j.cemconcomp.2022.104414