

Defne Circi

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EDUCATION	<p>Duke University, NC, USA <i>08/2022 - 05/2027 (Expected)</i> <i>Ph.D.</i>, Materials Science <i>MS</i>, Computer Science Advisors: L. Catherine Brinson Relevant Coursework: NLP, LLMs, Deep Learning, Computational Materials Science</p> <p>TU Delft, Delft, Netherlands <i>08/2019 - 01/2020</i> <i>Study abroad</i>, Technology, Policy, and Management Learning Highlights: Entrepreneurship, Economic Foundation, Ethics & Engineering Sabanci University, Istanbul, Turkey <i>08/2017 - 05/2022</i> <i>B.S.</i>, Materials Science & Computer Science GPA: 3.85/4.0 Relevant Coursework: AI, ML, Materials Characterization</p>
RESEARCH INTERESTS	<p>Natural Language Processing, Deep Learning, Comp. MatSci I am working on complex information extraction in science domains using language models and scientific reasoning models. I aim to process scientific articles at a scale and build materials databases that can be used to accelerate scientific discovery.</p>
RESEARCH EXPERIENCE	<p>AI & Materials Research Intern, IBM Research - CA/USA <i>05/2025 - 08/2025</i> Improved reasoning ability of chemistry language models by over 50% using reinforcement learning with verifiable rewards (RLVR), and applied for a patent on the proposed approach. Contributed to synthetic pretraining data generation and developed agent tools for chemistry question answering. Designed a benchmark and evaluation metric for PFAS regulation information extraction for the safe materials advisor model.</p> <p>Senior Graduation Project, Sabanci University - Turkey <i>08/2021 - 05/2022</i> Designed machine learning models (e.g., ridge regression, XGBoost) to predict concrete compressive strength, improving the prediction accuracy by 32%, and integrated predictive capabilities into a web app to support efficient processing and reduce experimental trial time.</p> <p>Research Intern, HZDR - Germany <i>08/2021 - 09/2021</i> Evaluated ML models to predict electronic structures from atomic configurations, achieving DFT-level accuracy with negligible computational cost by bypassing the $O(N^3)$ step, and tested model transferability across temperatures.</p> <p>Research Intern, Northwestern University - IL/USA <i>06/2021 - 07/2021</i> Improved impact mitigation performance of 2D elastic networks by embedding magnets and optimizing lattice design, resulting in a 15% increase in energy absorption efficiency, using LAMMPS MD simulations to model magneto-elastic interactions and simulate impact scenarios.</p>
SELECT PUBLICATIONS	<ol style="list-style-type: none">Circi, D., Bradley, M., Blouir, S. ..., Information Extraction from Diverse Charts In Materials Science, LM4Science Workshop at COLM, 2025.Ismayilzada, M., Circi, D., Jonne Sälevä, J., Sirin, H. ..., Evaluating Morphological Compositional Generalization in LLMs NAACL, 2025.Circi, D., Khalighinejad, G., Chen, A., Dhingra, B., & Brinson, L. , Extracting Materials Science Data from Scientific Tables Language + Molecules Workshop at ACL, 2024.

4. Khalighinejad, G., **Circi, D.**, Brinson, L. & Dhingra, B., [Extracting Polymer Nanocomposite Samples from Full-Length Documents](#) ACL, 2024.
5. **Circi, D.**, Khalighinejad, G., Chen, A., Dhingra, B., & Brinson, L. , How Well Do LLMs Understand Tables in Materials Science? IMMI, 2024.
6. **Circi, D.**, Khalighinejad, G., Badhwar, S., Dhingra, B., & Brinson, L. , [Retrieval of Synthesis Parameters of Polymer Nanocomposites](#), AI4MAT Workshop at NeurIPS, 2023.

GRANTS, AWARDS & HONORS

[Anthropic Award – LLMs for Materials Hackathon](#) 2024
 Developed MaSTeA, an interactive web app that enables easy testing of LLMs to evaluate their strengths and weaknesses across various subfields of materials science

[First Place – LLMs for Materials Hackathon](#) 2023
 Created InsightGraph, a tool that generates knowledge graphs from scientific article abstracts

[NSF aiM Graduate Traineeship and Fellowship](#) (full tuition support for 1 year) 2022
 Won third place in data science graduation project competition 2021
 Fulbright principal candidate for master's programs 2021
 TUBITAK Trainee Researcher Scholarship Program support for the COVID-19 project 2020
 Dean's High Honor List, Sabanci University 2017-2022
 Honor scholarship for 5 years (full tuition support) 2017-2022

CONFERENCE & WORKSHOP PRESENTATIONS

Materials Research Society Meeting, oral presentation, Boston - MA 12/2024
 Circi, D., Bradley, M., Dhingra, B. & Brinson, L. IE from Diverse Materials Science Charts

[South NLP Symposium](#), poster presentation, Atlanta - GA 04/2024
 Circi, D., Khalighinejad, G., Dhingra, B. & Brinson, L. How Well Do LLMs Understand Tables in Materials Science?

[Materials Research Data Alliance Annual Meeting](#), oral presentation, virtual 02/2024
 Circi, D., Khalighinejad, G., Dhingra, B. & Brinson, L. Using LLMs to Mine Materials Literature

[NeurIPS AI4MAT Workshop & ML4Molecules Workshop](#), poster presentation 12/2023
 Circi, D., Khalighinejad, G., Badhwar, S., Dhingra, B. & Brinson, L. Retrieval of Synthesis Parameters of Polymer Nanocomposites Using LLM

HIBIT, poster presentation (honorable mention), virtual 05/2021
 Azgari, C., Kilinc, Z., Turhan, B., Circi, D., & Adebali, O. The Mutation Profile of SARS-CoV-2 Is Primarily Shaped by the Host Antiviral Defense

TEACHING

TA, Data Science and Machine Learning for Science and Engineering, Duke University 2025
 TA, Structure and Properties of Solids, Duke University 2024
 TA, Computational Techniques for Materials at the Nano-scale, Sabanci University 2022
 TA, Introduction to Computing, Sabanci University 2021
 TA, Electrical, Optical & Magnetic Prop. of Materials, Sabanci University 2021
 TA, Computational Approaches to Problem Solving, Sabanci University 2020

RELEVANT SKILLS

Programming Languages and Tools: Python, Pytorch, R, C++
Spoken Languages: English (Professional), Turkish (Native)

OUTREACH & SERVICE

AI for Designing Materials Program guest speaker committee chair 2024-2025
 Reviewer for AI4MAT Workshop, ML for Life and Materials Science Workshop, Computational Materials Science, IMMI, Data in Brief

LLM Hackathon for Applications in Materials and Chemistry organizer 2024-2025
 NeurIPS Women in ML Workshop volunteer 2023