Defne Circi

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Education

Duke University, NC, USA *08/2022 - 05/2027 (Expected)*
Ph.D., Materials Science
MS, Computer Science
Advisors: L. Catherine Brinson
Relevant Coursework: NLP, LLMs, Deep Learning, Computational Materials Science

TUDelft, Delft, Netherlands *08/2019 - 01/2020*
Study abroad, Technology, Policy, and Management
Learning Highlights: Entrepreneurship, Economic Foundation, Ethics & Engineering

Sabanci University, Istanbul, Turkey *08/2017 - 05/2022*
B.S., Materials Science & Computer Science **GPA: 3.85/4.0**
Relevant Coursework: AI, ML, Materials Characterization

Research Interests

Natural Language Processing, Deep Learning, Comp. MatSci, Bioinformatics
I am working on complex information extraction in science domains using language models. I aim to process scientific articles at a scale and build materials databases that can be used to accelerate scientific discovery.

Research Experience

Senior Graduation Project, Sabanci University - Turkey *08/2021 - 05/2022*
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.

Research Intern, HZDR - Germany *08/2021 - 09/2021*
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.

Research Intern, Northwestern University - USA *06/2021 - 07/2021*
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.

Research Intern, TUBITAK *01/2020 - 05/2021*
Assigned previously identified clusters to SARS-CoV-2 genomes, visualized the clusters aligned with the phylogenetic tree; identified mutations per sample to understand the pathways and mutations of SARS-CoV-2.

Select Publications

1. Ismayilzada, M., **Circi, D.**, Jonne Sälevä, J., Sirin, H. ..., Evaluating Morphological Compositional Generalization in LLMs NAACL, 2025.
2. **Circi, D.**, Khalighinejad, G., Chen, A., Dhingra, B., & Brinson, L. , Extracting Materials Science Data from Scientific Tables Language + Molecules Workshop at ACL, 2024.
3. Khalighinejad, G., **Circi, D.**, Brinson, L. & Dhingra, B., Extracting Polymer Nanocomposite Samples from Full-Length Documents ACL, 2024.
4. **Circi, D.**, Khalighinejad, G., Chen, A., Dhingra, B., & Brinson, L. , How Well Do LLMs Understand Tables in Materials Science? IMMI, 2024.

5. **Circi, D.**, Khalighinejad, G., Badhwar, S., Dhingra, B., & Brinson, L. , Retrieval of Synthesis Parameters of Polymer Nanocomposites, AI4MAT Workshop at NeurIPS, 2023.
6. Jablonka, K.M., Ai, Q., Al-Feghali ..., 14 Examples of How LLMs Can Transform Materials Science and Chemistry: A Reflection on a LLM Hackathon Digital Discovery, 2023.
7. 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. Viruses, 2021.

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, Structure and Properties of Solids, Duke University *2024*
TA, Introduction to Computing, Sabanci University *2021*
TA, Electrical, Optical & Magnetic Prop. of Materials, Sabanci University *2021*
TA, Introduction to Data Science (High School Summer School), 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), **German** (Novice)

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*
NeurIPS Women in ML Workshop volunteer *2023*