Nofit Segal

(+1) 617-251-3911
nofit@mit.edu
nofitsegal.github.io
linkedin.com/in/nofit-segal

I am a PhD candidate working on machine learning methods for materials inverse design. My goal is to create tools that accelerate experimental materials discovery through predictive and generative modeling.

Education

MIT, DMSE & CSE — Cambridge MA, USA
MS/PhD in Computational Materials Science — 2022 - 2027 *(expected)*

- Eli and Dorothy Berman Fund Fellow, 2025-2026
- Google Schwarzman College of Computing Fellow, 2024-2025
- The Elie Shaio Memorial Award, 2023

Technion, Materials Science and Engineering — Haifa, Israel
BSc, Materials Science and Engineering — 2017 - 2022

- Rothschild Excellence Program Fellow, 2017-2022
- Dean's Excellence Award, 2019-2022
- Minor in Machine learning and Computational Science

Professional Experience

MIT, Learning Matter Group — Cambridge MA, USA
Graduate RA, P.I. Prof. Rafael Gomez Bombarelli — 2023 - 2027 *(expected)*

Technion, Electrochemistry and Energy Lab — Haifa, Israel
Undergraduate RA, P.I. Prof. David Eisenberg — 2020 - 2022

- Developed a 3D simulation to study percolation in a carbon-based porous electrocatalyst

Publications

Known Unknowns: Out-of-Distribution Property Prediction in Materials and Molecules
Nofit Segal*, *Aviv Netanyahu**, *Kevin P. Greenman, Pulkit Agrawal* †, *Rafael Gomez-Bombarelli* †. NPJ Computational Materials, 2025

- Spotlight talk in AI4Mat @ Neurips 2024, Materials Research Society (MRS) Fall Meeting, 2024

Lanthanoid coordination compounds as diverse self-templating agents towards hierarchically porous Fe–N–C electrocatalysts
Itamar Salton, Karina Ioffe, Tomer Y Burshtein, Eliyahu M Farber, Nicola M Seraphim, ***Nofit Segal****, David Eisenberg.* Materials Advances, 2022

Manuscripts in Preparation

The Loss Landscape of XRD-Based Structure Optimization Is Too Rough for Gradient Descent
Nofit Segal*, Akshay Subramanian, Mingda Li, Benjamin Kurt Miller, Rafael Gomez- Bombarelli.*

- AI4Mat @ Neurips 2025

Towards Generating Stable Materials via Large Language Models with Reinforcement Learning Finetuning
*Zhang-Wei Hong**, ***Nofit Segal****, Raina Wu, Aviv Netanyahu, Hoje Chun, Rafael Gomez-Bombarelli, Pulkit Agrawal.*

- AI4Science @ Neurips 2025

Learning Lattice Parameters from Powder X-Ray Diffraction Data Using Invariants
Elyssa Hofgard, Kyucheol Min, ***Nofit Segal****, Jigyasa Nigam, Tess Smidt*

- Predicting bispectrum coefficients from X-Ray Diffraction (XRD) patterns and inverting them to recover lattice parameters.

Projects

Extrapolation in Conditional Generation of Molecules
Generative Models course 6.S978, MIT 2024

Investigated out-of-distribution generalization in E(3)-equivariant molecular generation.

A Deeper Look into Equivariance for Materials Data
Advanced Deep Learning course 6.S989, MIT 2023

Implemented and trained E(3) Equivariant and non-equivariant GNNs for molecular energy prediction, comparing performance and latent geometry interpretability.

A Data-Driven Framework for Work Function Prediction Using Tree-Based Models
Undergraduate Senior Project, Technion 2022

Trained gradient-boosted trees for predicting work functions of solid materials, performing exploratory data analysis and feature importance analysis.

Sentence Transformer-VAE
Deep Learning course 046211, Technion 2022

Built a Transformer-based VAE for sentence generation, exploring reconstruction and latent space interpolation.

Service & Leadership

3rd Annual LLM Hackathon for Materials & Chemistry
MIT Site Organizer and Hackathon Judge 2025

MIT ESOL
Tutoring English for MIT service employees 2022 - present

MIT CSE Student Board
Treasurer 2022 - present

Rabin Leadership Program
Participated in the establishment of an after-school center for children 2012 - 2013