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

# 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.

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## 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 Future Research Cohort Fellows, 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 at AI4Mat at 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.*

- Oral Presentation at AI4Mat at 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 at 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