NOFIT SEGAL

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EDUCATION

MIT, DMSE & CSE Cambridge MA, USA
MS/PhD in Computational Materials Science 2022 - 2027 *(expected)*
- Google Schwarzman College of Computing Fellow, 2024
- 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

PUBLICATIONS

Known Unknowns: Out-of-Distribution Property Prediction in Materials
Nofit Segal*, Aviv Netanyahu*, Pulkit Agrawal†, Rafael Gomez-Bombarelli†. in submission
- Spotlight talk in AI4Mat @ Neurips, Materials Research Society (MRS) Fall Meeting, '24

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

PROFESSIONAL EXPERIENCE

MIT, Learning Matter Group Cambridge MA, USA
Graduate RA, P.I. Prof. Rafael Gomez Bombarelli 2023 - 2027 *(expected)*
- Materials discovery and inverse design using
  (1) Extrapolation in materials property prediction
  (2) Multimodal representation learning and generative modeling

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

PROJECTS

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

Explored OOD generalization abilities in conditional generations of molecules of an E(3) Equivariant Diffusion model.

A Deeper Look into Equivaraince 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.

Volunteering	**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