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

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

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