Noam Gamburg

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Education | GPA: 3.9/4.0

University of Illinois Urbana-Champaign **Champaign, IL**
Bachelor of Science in Chemical Engineering | Minor - Materials Science and Engineering Expected: **May 2028**
Accolades: National Chemistry Olympiad Finalist (Israel), Award for Academic Excellence - Open University of Israel

Technical Skills

Molecular & Materials Simulation: LAMMPS, GROMACS, VMD, OVITO, Avogadro, DFT, Gaussian, ORCA, RDKit, GNN/GCN, Polymer/ceramic/glass modeling, nanoparticle and biomolecular simulations
Programming/Automation & Materials: FTIR, TGA, DSC, SEM, XRD, DMA, Java, Python, CUDA, PyTorch, PyTorch Geometric, Git, MATLAB, Pandas, Bash, Linux/Unix, HPC, NumPy, SciPy, mechanical testing, JMP, high-throughput production pipelines
Visualization/Design & Technical Skills: Autodesk Maya, Houdini, Blender3D, Fusion360, Unreal Engine, GPU-accelerated visualization, procedural pipelines, scientific visualizations, Cross-functional collaboration, technical reporting, experimental/computational integration, hard-surface modeling, subD modeling, French/Hebrew/English Native

Experience

Jun Laboratory - Research Assistant — September 2025 - Present

- Developing and **training machine-learning models** in PyTorch Geometric to predict physicochemical properties of organic molecules, enabling data-driven optimization and prioritization of chemical tool candidates
- Applying density-functional theory (DFT)-based electronic structure calculations to model molecular properties, integrating Avogadro, ORCA, and Gaussian into reproducible computational workflows
- Synthesizing and experimentally characterizing organic compounds to validate computational predictions

Computational Visualization & Design Consultant — November 2023 - Present

- Delivering high-fidelity 3D product visualizations and design solutions for **50+ international clients** via contract-based engagements using procedural graphics pipelines and hard/subdivision-surface modeling techniques
- Collaborating with multidisciplinary design and engineering teams from Alfano, Teva, Ejer Paris, and the French National Energy Exhibition on technically constrained visualization and prototyping projects
- Designing procedural production pipelines for scalable product prototyping and visualization

Society For Biomaterials - Founder & Chapter President — October 2025 - Present

- Founded and currently leading the establishment of the UIUC chapter for the Society For Biomaterials, establishing its mission, structure, and programming around biomaterials research, design, and translational applications
- Recruiting, Interviewing and managing the **fastest growing membership** for organizations at UIUC with 30+ undergraduate/graduate students and faculty
- Coordinating with faculty and industry reps to develop research-focused events, lab tours, networking events, etc

Projects

Graph Neural Network - Computational Chemistry — October 2025 - December 2025

- Designed and implemented a full molecular generation and optimization pipeline using RDKit and PyTorch Geometric, programmatically enumerating and sampling Quinoline derivatives using node-edge tensors across multi-site functionalization spaces (>50,000 Quinoline samples used for training)
- Developed a Graph Neural Network (GNN) operating directly on molecular graphs, encoding physicochemical features to predict LogP with end-to-end differentiable learning
- Applied model to **>50 billion molecular combinations**, ranking synthetically feasible candidates based on predicted logP

Computational Molecular Dynamics - App Development (Python & CUDA) — March 2025 - June 2025

- Architected and implemented a modular Python application for physics-based molecular dynamics simulation orchestration, abstracting low-level command prompt configuration and file management into **vastly improved workflow efficiency** with much greater accessibility
- Developed AI-enhanced automation pipelines for simulation setup, including data-driven selection and optimization of simulation parameters, timestep controls, and LAMMPS run configurations
- Integrated GPU-accelerated computing via CUDA to enable scalable, high-throughput molecular simulations and post-processing of atomistic trajectory data

Independent Computational Molecular Dynamics Research — September 2024 - Present

- Designing, parameterizing, and executing molecular and biomolecular simulations using LAMMPS, GROMACS, and ORCA, spanning classical MD and quantum-chemistry-based calculations
- Investigating nanoparticle stability and protein denaturation through analysis of structural and thermodynamic behavior across simulated conditions
- Applying advanced scientific visualization (Houdini, Maya, OVITO, VMD) to interpret and more effectively communicate complex molecular dynamics results