

Lab Engineer/Research Associate in Machine Learning for Chemistry

Poranne Lab, Schulich Faculty of Chemistry, Technion – Israel Institute of Technology

Appointment: Full-time

Start date: Flexible (preferably by early 2026)

About the Lab

The **Poranne Group** is a computational physical organic chemistry group that develops and applies machine learning methodologies to advance discovery and understanding in chemistry. Our research focuses on **interpretable deep learning, molecular representations, and chemistry-aware models** that connect data-driven insights with fundamental chemical understanding. The group operates at the interface of **computational organic chemistry, machine/deep-learning, and data science**. For more information, visit our website: <https://poranne-group.github.io/>.

Position Summary

We are seeking a highly motivated **Lab Engineer/Research Associate** to take a leading role in our lab's research activities. The successful candidate will be responsible for **developing and applying machine learning models for molecular and physical systems** and **training graduate and undergraduate researchers**.

Key Responsibilities

- Conduct collaborative research in machine learning for chemistry and materials.
 - Develop interpretable ML architectures and model analysis tools for scientific data.
 - Supervise and train graduate students and contribute to their technical and professional development.
 - Assist in the writing of research articles, technical reports, and grant proposals.
 - Contribute to data curation, model implementation, and computational infrastructure management.
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Essential qualifications:

- M.Sc. or Ph.D. in Computer Science, Computational Chemistry, Bioinformatics, Physics, or a related field.
- Strong proficiency in Python and key ML/scientific libraries (PyTorch, JAX, TensorFlow, NumPy, pandas, PyTorch Geometric, RDKit, etc.).
- Solid understanding of software engineering best practices (version control, testing, packaging, CI/CD).
- Experience with DevOps/MLOps tools (including Docker, Kubernetes, MLflow, DVC, etc.).
- Demonstrated experience applying ML to scientific or engineering data (e.g., molecular simulations, protein structures, reaction networks, spectroscopy, materials data).
- Comfortable working in Linux-based development environments and with cloud/HPC systems.

Preferred qualifications:

- Experience with AI models for molecules or materials (e.g., graph neural networks, equivariant networks, molecular transformers).
 - Familiarity with scientific data formats and repositories (PDB, PubChem, ChEMBL).
 - Exposure to computational chemistry or structural biology workflows.
 - Contributions to open-source scientific software or AI toolkits.
 - Strong cross-disciplinary communication skills and intellectual curiosity.
 - Experience mentoring students or coordinating research teams.
 - Interest or experience in scientific writing.
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What We Offer

The Schulich Faculty of Chemistry provides a vibrant and collaborative research community at one of Israel's leading scientific institutions.

The Poranne Group offers access to state-of-the-art computational resources and a strong network of collaborations across chemistry, physics, and computer science. Our group provides a supportive and intellectually stimulating atmosphere, emphasizing creativity, rigor, and teamwork. In our group, you will enjoy the chance to shape next-generation tools to address problems at the intersection of AI, theory, and experiment, as well as the freedom to explore creative research directions aligned with the lab's mission.

Salary will be commensurate with qualifications and experience, following Technion guidelines.

How to Apply

Interested candidates should submit the following materials to Prof. Renana Poranne at rporanne@technion.ac.il:

- A cover letter describing research interests, experience, and motivation.
- Curriculum vitae (including publications).
- Contact information for two or more references.

Applications will be reviewed on a rolling basis until the position is filled.