



## Differentiable molecular dynamics simulations of non-equilibrium biomolecular systems

*[Engel Research Group](#) at the University of Calgary*

**Preferred Start:** Fall 2026

**Application Deadline:** **January 25** for consideration for funding from the prestigious [Canada Impact+ Research Training Awards](#) (international students applying for PhD level only); otherwise **May 1, 2026**

**Supervisor:** Dr. Megan C. Engel, Assistant Professor, Biological Sciences Department, University of Calgary ([megan.engel@ucalgary.ca](mailto:megan.engel@ucalgary.ca))

### Description

The Engel Research Group is recruiting outstanding candidates for graduate student positions, 2 at the Masters level and 1 at the Doctoral level, to pursue interdisciplinary research at the intersection of biology, chemistry, physics, and machine learning. The overarching foci of the group are (i) to elucidate how naturally evolved systems have taken advantage of nonequilibrium physics to excel at their biological functions and (ii) to develop rational design principles for *de novo* nucleic acid and protein nanotechnology. To achieve these ends, the Engel Group harnesses advances in the hardware and software that undergird modern machine learning – particularly, automatic differentiation – to develop improved biomolecular models; perform innovative optimizations over molecular dynamics simulations of DNA, RNA, and proteins; and interface non-equilibrium physics theories with biological systems.

### Available projects include:

- Investigating the optimality of the ATP synthase molecular motor through multi-scale differentiable molecular dynamics simulations;
- Elucidating control mechanisms for the epithelial-mesenchymal transition in cancer cells through differentiable molecular dynamics simulations and gene network modelling;
- Inverse design of external control protocols and active particle interactions to control spatiotemporal patterning in active matter systems;
- Contributing to the development of [in-house software](#) for improving biomolecular modelling according to the machine learning paradigm;
- Developing coarse-grained models of peptide nucleic acids (PNAs) in collaboration with experimentalists, using [in-house software](#).

The specific project will be refined from the above options according to the candidate's interests and background. **Work in the Engel lab is fully computational/theoretical** with opportunities for close collaboration with experimental groups. The Engel group has dedicated, priority access to substantial HPC hardware including seven H100 GPU units. A document outlining what you can expect while working in the Engel lab can be found [here](#).

The University of Calgary is committed to an equitable, diverse, and inclusive workforce. We welcome interest from all qualified persons. We encourage women; First Nations, Métis and Inuit persons; members of visible minority groups; persons with disabilities; persons of any sexual orientation or gender identity and expression; and all those who may contribute to the further diversification of ideas and the University to apply.

## Requirements

### Essential

- A four-year baccalaureate degree or equivalent from a recognized institution.
- A minimum of 3.2 GPA on a 4.0-point system (or equivalent) over the past two years of full-time study
- C1-level English proficiency (CEFR framework)
- Interest in computational biophysics
- **If interested in applying for the prestigious [Canada Impact+ Research Training Awards](#) (CIRTA), applicant must not be currently based at a Canadian institution**

### Desirable

- Prior coursework and/or research experience in physics, computer science, and/or numerical methods
- Programming experience (Python preferred)
- BSc degree in physics, biological sciences, computing sciences, computer engineering, natural sciences or any other relevant quantitative fields.

## Additional Details

**Location:** University of Calgary, Calgary, Alberta, Canada

**Salary (Guaranteed Minimum):**

	Domestic	International	International with CIRTA award
Year 1	\$33,000 CAD	\$34,000 CAD	\$42,550 CAD
Year 2	\$33,600 CAD	\$35,700 CAD	\$44,250 CAD
Year 3	\$34,500 CAD	\$36,600 CAD	\$45,150 CAD
Year 4	\$35,100 CAD	\$37,500 CAD	\$46,050 CAD

**Benefits:** Health and dental benefits are provided for an annual fee through the [Graduate Students' Association Health and Dental Plan](#).

More information about graduate studies in the Department of Biological Sciences at the University of Calgary can be found [here](#).

## Application

Please email the following to [megan.engel@ucalgary.ca](mailto:megan.engel@ucalgary.ca):

- A recent transcript (unofficial is fine)
- CV/resume
- Names and contact information for 2-3 references
- Brief (100-200 words) statement outlining why you are interested in researching in the Engel lab