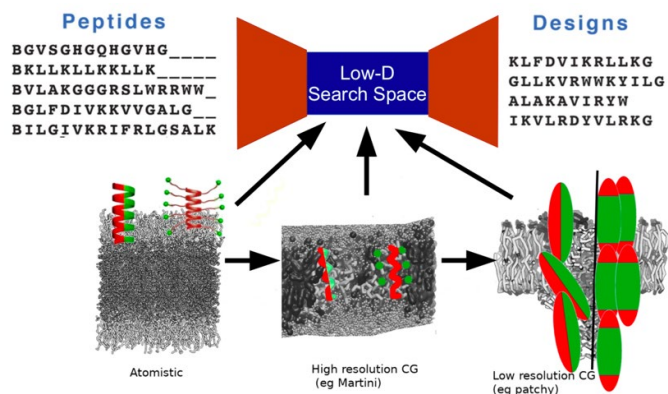# Graduate student position will be available, starting in the Fall 2021 / Winter 2022, in the group of Professor Rachael Mansbach
Department of Physics, Concordia University, Montreal, Canada.

Proteins are the building blocks of living things, miniature motors that make all of your cells function. Proteins embedded in cell membranes filter out toxic materials or uptake necessary nutrients. Meanwhile, malfunctioning proteins are responsible for a slew of disorders, including Alzheimer's, type II diabetes, and Parkinson's. Therefore, it is of great interest to be able to study the molecular mechanisms of various proteins, either to correct when things go wrong, or to design drug molecules to inhibit the proteins of damaging cells such as bacteria or cancerous cells.

My primary scientific interests lie in designing small molecules and peptides (short proteins) for therapeutic applications: killing bacteria and drugging human cells in beneficial ways—for example to find new analgesics for treatment of chronic pain disorders, or to correct dysregulation of pathways involving the intrinsically disordered proteins that lead to Alzheimer's. In order to do this, I employ theoretical and computational biophysics tools. I am particularly interested in the burgeoning field of deep learning as applied to molecular dynamics and drug design. Over the past decade, generative deep learning (training an AI to create by pattern-matching to a large amount of data) has demonstrated a fascinating ability to create images and text, and there has been an explosion in the past three years over its application to drug design and molecular dynamics, but it still suffers from lack of interpretability and scalability. As a physicist, I am particularly interested in the interpretability issue.

Theory of disulfide bonds for toxin-based therapeutics
Due to their high specificity and binding affinity for various receptors involved in different biological pathways, toxins have for a long time been considered a rich natural source of therapeutic. A large and intriguing class of toxins is those that are short, cysteine-rich peptides whose structures are largely controlled by the multiple disulfide bonds that form between the cysteines. Historically, one difficulty in assessing the structure and hence the proposed mechanisms of such toxins has been that it can prove difficult to controllably fold them to their native stable states *in vitro*. Indeed, there is evidence that certain toxins exist even *in vivo* in metastable states that are nonetheless potent, and in certain cases the "non-native" fold demonstrates higher selectivity and binding affinity which leads to the question of whether we can control these metastable states through sequence, environment, or kinetic engineering. I am looking for a student interested in either polymer theory or molecular dynamics, to explore ways to bring together constrained polymer theories with bond-breaking force field models to map out the free energy landscapes of disulfide-rich toxins.

Desired qualifications. I am looking for strongly-motivated graduate student candidates interested in theoretical biophysics and deep learning. Physics or Biophysics BA or BS is preferred but I am happy to take CS, biomedical engineering or related fields if the match is good. Experience with coding will be valuable, particularly in Python, and prior experience with molecular dynamics simulations will also be useful. I would like to cultivate an ***inclusive, diverse and collaborative*** lab environment and I would particularly like to encourage members of traditionally underrepresented groups in STEM to apply. I am happy to work with students on their own ideas—as long as they fall within the broad scope of my work—and/or to tailor projects to suit specific strengths and interests.

Concordia Department of Physics is a growing department in a university with rapidly increasing rating. We offer research-based M.Sc. and Ph.D. programs. Our faculty members conduct research in the areas of Condensed Matter Physics (theoretical and experimental), Molecular Biophysics, Medical Physics / Imaging, Photonics, Theoretical High Energy Physics, Computational Physics and Physics Education.

Successful applicants will be offered financial packages consisting of RA, TA and various awards of at least 20,000 CAD per year (often more), for 4 years (Ph.D.) or 2 years (M.Sc.). International students will be offered tuition remissions or other awards to compensate for the international tuition fees.

Please contact Professor Rachael Mansbach (re.mansbach@concordia.ca) or Valter Zazubovits (valter.zazubovits@concordia.ca; Graduate Program Director) for more information.