Vita

Candidate's name: Emily Claire Anderson

Universities Attended:
University of New Brunswick (2021)
Bachelor of Science
Honours

University of New Brunswick (2024)
Masters of Science

Conference Presentations:

"Machine learning towards automated discovery of organic molecules for use in non-aqueous redox flow batteries" E. C. Anderson, S. De Baerdemacker, and A. El-Samman, CSC Canadian Chemistry Conference and Exhibition 2022, Calgary, AB, June 2022 (Poster).

"Machine learning towards automated discovery of organic molecules for use in non-aqueous redox flow batteries" E. C. Anderson, 2nd workshop of AARMS CRG on Mathematical Foundations of Scientific Machine Learning, Fredericton, NB, August 2023 (Talk).

Machine Learning Towards Automated Discovery of Organic Molecules as Active Materials in Non-Aqueous Redox Flow Batteries

UNIVERSITY OF NEW BRUNSWICK

THESIS DEFENCE AND EXAMINATION

in Partial Fulfillment

of the Requirement for the Degree of
Master of Science

by

E. Claire Anderson

in the Department of Chemistry

U.N.B., Fredericton, N.B.

Thursday, May 23rd, 2024
10:00 a.m.

Toole Hall, Room 303

Examining Committee

Dr. Stijn de Baerdemacker	Supervisor
Dr. Anna Ignaszak	Internal Examiner
Dr. Gobinda Saha	Int-Ext Examiner
Dr. Gilles Villemure	Chair of Oral Examination

Abstract

With the increasing demand for energy and the resources needed to provide this energy, redox flow batteries (RFBs) have shown potential as highly flexible large-scale energy storage systems. These electrochemical energy storage systems make use of redox processes for the conversion of electrochemical energy and are highly appealing due to the ease of their scalability to fit the size necessary for many energy storage applications. In this project, interest lies in the automated discovery of organic redox active materials that are able to undergo both oxidation and reduction reactions for use in symmetric non-aqueous RFBs. Machine learning methods have been applied to automate the process of generating unique organic molecules from given parameters followed by attempts to improve the generated data set through the application of a genetic algorithm (GA). The initial set of molecules were constructed through a series of random choices under set structural parameters based on an unsubstituted bipyridine backbone. The molecules were characterized computationally through a series of calculations to determine their redox and cell potentials, stability, and solubility and then ranked based on these values to select the population that will be run through a GA that was designed to combine the structural features of two randomly chosen molecules from this population to generate new molecules for future GA generations. A set of top ranking molecules have been determined as good candidates for use in non-aqueous RFBs.