

Annual Progress Report 2025–2026

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I began my Ph.D. studies in the Department of Chemistry at the University of Toronto in September 2025. My studies and research in Toronto have been generously supported by the Shida Scholarship. In this report, I summarize my first year, including my coursework, research progress, and life in Toronto.



University of Toronto

Coursework

In the Ph.D. program in theoretical chemistry at the University of Toronto, students are required to complete six graduate-level courses before obtaining their degree. During my first year, I completed three of these courses: a course in quantum mechanics (CHM1478H), a course in statistical mechanics (CHM1480H), and a course on machine learning for chemistry (CHM1449H). The quantum mechanics and statistical mechanics courses each consisted of two hours of class per week, while the machine learning for chemistry course consisted of three hours per week.

Since I had not taken equivalent graduate-level courses in quantum mechanics or statistical mechanics at Kyoto University, I initially spent a considerable amount of time working on the assignments for these courses. However, both classes provided fundamental knowledge that is closely related to the core of my current research, and I found them extremely valuable. In the machine learning for chemistry course, I learned not only how machine-learning methods can

be applied to chemistry, but also how the resulting models and predictions can be interpreted from physical perspectives. At first, I also found it challenging to balance research with coursework and to follow specialized lectures in English, but I gradually became accustomed to both.

In addition, graduate students in physical chemistry attend a weekly seminar series. These seminars include research presentations by graduate students in physical chemistry as well as lectures by invited professors from outside the university. This provides opportunities to learn about a broad range of research topics in physical chemistry beyond my own area of specialization. Ph.D. students are also required to give two seminar presentations on their own research before completing the degree.

Research

I joined the research group of Prof. Anatole von Lilienfeld. The group holds a weekly group meeting, as well as several one-hour morning meetings each week. Rather than working mainly on large collaborative projects, members of the group generally pursue their own independent research projects.

My research project focuses on the development of new quantum-chemical methods using machine learning. In recent years, artificial intelligence has been increasingly applied in chemistry. Many of these applications rely on large amounts of data generated by quantum-chemical calculations. However, quantum-chemical methods generally involve a trade-off between computational cost and accuracy, which remains an important challenge.

My research aims to address this issue by incorporating machine learning into quantum-chemical calculations to achieve higher accuracy while maintaining relatively low computational cost. During my first year, I obtained several promising results indicating the potential of the proposed approach. I plan to continue developing and validating the method for a broader range of chemical systems.

Life in Toronto

Life in Toronto has been a very positive experience. One of the aspects I particularly appreciate is the city's cultural diversity. People from many different countries live in Toronto, and this diversity is strongly reflected in its restaurants and food culture, making it possible to enjoy cuisines from all over the world within the city. Perhaps partly because of this multicultural environment, I have also found people in Canada to be very understanding toward non-native English speakers. Even when I have difficulty expressing myself clearly in English, many people are patient, listen carefully, and make an effort to understand what I am trying to

say. This has given me the impression that Toronto is a very welcoming place for people from abroad.

Toronto is also a very comfortable city in the summer, with relatively mild temperatures and many opportunities to spend time outdoors. In contrast, the winter was colder than I had expected before coming to Canada, and going outside can be difficult on particularly cold days. However, buildings in Toronto are generally very well heated, and I often find indoor environments more comfortable in winter than those in Japan.

During weekends and holidays, I was able to refresh myself by spending time in nature and enjoying activities outside of university. I visited Niagara Falls with friends and went camping in areas surrounded by nature. I also had the opportunity to enjoy the excitement surrounding major sporting events. The Blue Jays advanced to the World Series last year, and Canada was one of the host countries of the FIFA World Cup this year, which created a lively atmosphere throughout the city.

In addition, Ms. Rika Okayama, the former Executive Director, kindly hosted two dinner gatherings with her family and Mr. Mukumoto, a recipient of the 2025 Shida Scholarship Program. I greatly enjoyed both occasions and appreciated the opportunity to spend time with them. I would like to thank Ms. Rika Okayama for organizing such wonderful dinner gatherings.



Niagara Falls



Blue Jays game



First dinner gathering



Second dinner gathering

Acknowledgment

I would like to express my sincere gratitude to the Shida Scholarship Program, the Shida family, and Kyodai Collaborative for their generous financial support of my doctoral studies at the University of Toronto. I would also like to thank Ms. Rika Okayama and Ms. Nanako Tojo for their kind assistance with various administrative matters. Thanks to their support, I have been able to focus on my research and academic work while also gaining the valuable experience of living and studying abroad. I hope to make the most of my time in Canada and continue to grow not only as a researcher, but also as a person.