

# PhD or MSc position in theoretical chemistry at the University of New Brunswick

The QuNB group of Stijn De Baerdemacker (Canada Research Chair, Tier 2 in Theoretical Chemistry) from the Department of Chemistry at the University of New Brunswick (Canada) has a position for a PhD student available starting May or September 2020.

Research in the QuNB group is situated around the development of electronic structure methods for finite-size and strongly correlated quantum many-body systems. Major research themes consist of geminal theory, beyond-integrability methods, density-matrix approaches, machine-learning methods, among others. More information on our research projects can be found on the [website](#) of the group.

Solving the quantum many-body problem remains one of the key challenges for the future. Many of the solutions to today's technological, medical and societal problems will be found in tomorrow's smart devices, molecules and materials. Therefore, it is of utmost importance that we develop those theoretical and computational tools that will allow us to understand and predict the quantum properties driving those materials. Machine Learning methods are emerging as a new tool to provide accurate predictions for quantum mechanical observables. However, the inner workings of these methods however often remain mysterious, as it is not always clear how they arrive at a certain prediction. The purpose of this PhD project is to investigate the interpretability of Machine Learning methods for quantum chemistry.

The PhD student will be directly involved with the development of (a) new Machine Learning methods for the quantum many-body problem, and (b) the tools to grasp a better understanding of the inner workings of these methods. The project will combine fundamental theoretical work with the implementation into efficient computational codes. The student will be able to enjoy access to high performance computing facilities and a strong international collaboration in North America and Europe.

Interested applicants should be holder of a degree in chemistry, physics, mathematics or computer science, and be highly motivated to work in an interdisciplinary environment. Strong knowledge of quantum many-body theory, quantum chemistry or machine learning is an asset. Preliminary inquiries should be directed to [stijn.debaerdemacker@unb.ca](mailto:stijn.debaerdemacker@unb.ca) and should include a motivation letter and current CV. Formal applications must be processed and completed online at <https://apply.unb.ca>. Applications will be reviewed until the position is filled.

Established in 1785, the University of New Brunswick is one of North America's oldest public universities. UNB's outstanding quality and breadth of teaching, ranked areas of study, relevant research and innovative programs make it a leading national university. UNB has two main campuses, with a total enrollment of 12,000 students from more than 100 countries. Both campuses offer the comfort and security of a small community with the vibrancy of a bigger city. The Fredericton campus, one of the most beautiful in the country with its red brick, ivy-covered Georgian architecture and lush landscape, is located in the capital city, which has been ranked as one of the best places to live in Canada.