GTR Interdisciplinary Research Report
Quantum Simulation Technologies, Inc. (QSimulate)

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Affiliation:

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Academic Year: 3rd Year in Ph.D. Program

Destination: Quantum Simulation Technologies, Inc. (QSimulate) in Boston, MA

Period: August 2023 – October 2023

Purpose:

Acquiring Advanced Computational Methodologies for Quantum Chemistry Held by QSimulate

■ Summary:

There are many challenges in computational quantum chemistry such as determination of the global minima (GM) in the potential energy surface (PES) of the micro-solvated molecular cluster, identification of the transition state (TS) structure in the chemical reaction of interest, and generation of the well-defined internal coordinate of the molecular systems. During this overseas study, I attempted to overcome these challenges by combining or modifying more than 10 program modules written in Python or C++. Also, I've written automated programs to make complex procedures easy to follow, use and analyze. Sometimes there is no documentation for program usage and installation guidelines. In addition, some programs cannot be applied to the molecules of interest because the systems being investigated have unique electronic structures. However, even if such cases, I could successfully specify the problematic lines in source code and fix the problem by reading the published papers and checking the source code thoroughly, or work together with colleagues in QSimulate. Finally, with in-depth discussions with QSimulate members, I resolved the challenges written above to some extent. Through this study abroad for 3 months, I got many experiences and advanced techniques for quantum chemical calculations, and improved my programing skills greatly.

■ Impressions:

➢ Research:

In QSimulate, I've learned (1) one of the algorithms for finding the GM of the solvated molecular cluster, which is easy to implement, (2) sophisticated TS search techniques and protocols at a low cost, (3) how to define correct internal coordinates of the molecules, (4) the power of modern and cutting-edge semi-empirical quantum chemical calculation methods, (5) program automation of the workflow. In my Ph.D. research, I applied several of these methods and also created an

efficient code generator program, getting some favorable descriptions of the molecular properties under study, which would have been definitely unattainable without QSimulate. As for programing skills, I've read many source codes of the quantum chemical calculation tools more intensively over a short period than before, and modified those as required, leading to faster programming on my part. I would like to utilize the skills gained through this interdisciplinary research in my ongoing Ph.D. study.

- Environment:

Boston has a milder climate in summer compared to Nagoya, making it comfortable to live in; however, the same cannot be said for winter because the temperature is expected to drop below freezing. As for the appearance of the city, it is neat especially for the vicinity of Harvard Square. The only slightly disappointing thing is the presence of a fair number of homeless people and beggars, although I suppose it is a part of diversity. Of course, the cost of living is very high, and it is even considered the most expensive city in the U.S.

In QSimulate, my colleagues usually arrive at the office at 9-10 a.m. and leave work at 5-6 p.m., so I followed suit and did the same. The office building was very tidy and clean. Since it has a cafeteria inside (**Figure 1**) and there is also a famous grocery store nearby, I didn't have any trouble finding lunch. Anyway, during the life in this short-term visit, there wasn't any particular inconvenience, and I enjoyed the research in QSimulate very much.

■ **Acknowledgement:**

I would like to express my gratitude to the GTR Program for providing me with the opportunity to engage in interdisciplinary research in Boston. I also would like to extend my thanks to Ms. Ando in GTR Student Support Office and Ms. Yamada in Quantum Chemistry Laboratory for handling some complex financial and administrative procedures on my behalf. Finally, special thanks go to Dr. Toru Shiozaki, CEO of QSimulate, for allowing me to study in his company.

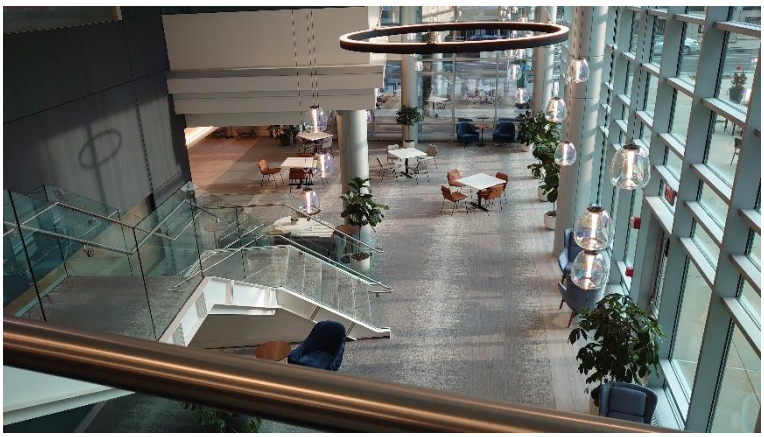

Figure 1. The cafeteria inside the office building