（別紙様式５）

# 変革を駆動する先端物理・数学プログラム（FoPM）

## 国外連携機関長期研修　報告書

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I participated in an internship at the Japan office of Classiq Technologies for one month, throughout February 2026.

**Background and Objectives of the Internship**

My research has focused on simulating first-quantized Hamiltonians on quantum computers. Some methods for executing these simulations require performing arithmetic operations on a quantum computer, which led me to be interested in software that can easily implement such quantum circuits. "Qmod," offered by Classiq Technologies, is precisely that kind of software. I previously had the opportunity to use the Classiq platform after being granted a trial license. Following this, Classiq Technologies reached out to me for feedback on the software. Through our subsequent technical exchanges, they inquired about my interest in an internship. Since Qmod is one of the few software tools aiming to be a high-level language for quantum programming, and because the internship offered the invaluable opportunity to work directly with the Qmod development team at their Japan office, I decided to participate.

**Work Performed During the Internship**

During my internship, I developed two demonstration Jupyter Notebooks for Classiq's official documentation. A key feature of Classiq's software is "QNum," which treats multiple qubits as numbers represented in binary. This functionality significantly simplifies the construction of quantum circuits, particularly when performing arithmetic operations on a quantum computer. While QNum has primarily been utilized for creating oracles in Grover's algorithm or implementing Quantum Singular Value Transformation (QSVT), there were previously no documented examples of its application in the field of quantum chemistry. I explored and developed practical examples of how QNum can be applied to chemistry-related problems and provided these implementations for the platform's documentation.

As one example, I implemented a Jupyter Notebook that demonstrates the calculation of the ground-state energy for the Quantum Drude Oscillator (QDO) model using the Variational Quantum Eigensolver. Intermolecular dispersion forces can be determined by calculating the interaction between two molecules; however, the total force does not simply triple when a third molecule is introduced. This phenomenon is referred to as many-body dispersion. While it is desirable to evaluate dispersion forces using first-principles calculations, attempting to do so for multiple specific molecules results in an exorbitant increase in computational complexity. The QDO model [1] is a coarse-grained model that describes "molecules interacting via dispersion forces" as "electrostatic interactions between QDOs." In this model, a QDO is defined as a harmonic oscillator consisting of a pair of fictitious positively and negatively charged particles connected by a spring. QDOs behave as bosons, and in the Jupyter Notebook, I showed how we can treat such a bosonic system using the classiq package [2]. In representing the QDO system, we utilize Fock states, which are basis states that specify the number of particles, or occupancy, in a given energy level. Unlike a two-level qubit system limited to 0 and 1, a bosonic Fock state is characterized by non-negative integer values ($n = 0, 1, 2, \ldots$). Consequently, representing these states on a quantum computer involves multi-bit registers to encode these integers. This makes the model particularly well-suited for QNum, as it enables seamless integration of multi-bit integer representations into quantum algorithms.

Another implemented example is a simulation of excitation energy transfer based on a continuous-time quantum walk. Photosynthesis is the process by which plants use light energy to synthesize organic compounds from carbon dioxide and water. During this process, pigment-protein complexes known as light-harvesting complexes absorb light energy or receive it from other complexes, transporting this excitation energy to a reaction center. The most critical aspect of this process is the energy transfer mechanism. It is experimentally known that

quantum interference plays a role in this mechanism, and one of the light-harvesting complexes where such phenomena have been observed is the Fenna-Matthews-Olson (FMO) complex [3]. The FMO complex has a trimeric structure, with each subunit containing eight Bacteriochlorophyll *a* pigments. Seven of these are strongly bound within the protein scaffold and interact with each other due to their arrangement within the scaffold [4]. It is well established that the optical spectra of the FMO complex are primarily determined by the interactions within a single subunit [5]. For the simulation, an excited state localized on a single pigment (a Frenkel exciton) was represented as an integer from 0 to 6. Leveraging the compatibility of this encoding with QNum, I implemented a continuous-time quantum walk in the Jupyter Notebook using the Frenkel exciton Hamiltonian given in [5].

**On-site Experience**

The Classiq Japan office is located in the Shin Marunouchi Building, offering a panoramic view of Tokyo Station. During my time there, the engineers at Classiq Japan were incredibly supportive, providing detailed guidance not only on technical coding questions but also on presentation techniques for non-technical audiences.



Figure 1. Exterior view of the Japan office of Classiq Technologies

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