# Experience Report

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HQS Quantum Simulation GmbH, located in Karlsruhe, Germany, is a company that develops quantum simulation software for drug discovery and chemical development. HQS offers software that can readily be run on/via quantum computers, classical hardware, or the company's cloud service QAD cloud. The company was founded in 2017 by researchers from the Karlsruhe Institute of Technology, and currently it has 30 employees. It has customers from the chemical and material industry, such as Bosch, BASF, and Merck.

The R&D infrastructure in HQS is divided into three roadmaps — Quantum Computing, Ab-initio Calculations, and Lattice Systems. The three roadmaps account for different aspects that need a work to be combined into future products. The workflow at HQS is split into two-week "sprints", which is in general a scrum structure. On the first day of the sprint, employees plan their work for two weeks. Also, there is an all-company meeting on this day, where the announcements are made for all employees. Once a week, there is a meeting with the roadmap leader to discuss the work progress and the next steps in detail. Over the week, there is a daily meeting for every roadmap team, in which the employees briefly present their work on the previous day and their plan for the day. The daily meeting can also be used to ask short questions or discuss who to approach with a problem to avoid getting stuck. On the last day of the sprint, employees also present their reflection on their sprint during the daily meeting. The last day of the sprint is called "freaky Friday", where the employees can work on and explore self-chosen topics not directly related to their ongoing project at HQS. In addition, there is an HQS seminar every Friday, where the researchers from within or outside HQS are invited to speak about their work. The interns follow the same workflow. The IT infrastructure involves Mattermost (internal communication), Gitlab (code and text documentation), Nextcloud (slides and project documentation), Jira (project/task planning), and Confluence (wiki and other organizational documentation).

I worked at the Quantum Computing team under the supervision of Dr. Jan Reiner, for three months. My work, as a software developer, was to investigate the efficiency of the tket quantum compiler and develop an interface between tket and HQS' software stack. The purpose of the compiler is (i) to translate the circuit into a form which is executable on a quantum backend, and (ii) to optimize the circuit to minimize the circuit size. The efficient compilation is particularly important if the circuit is executed on NISQ devices — devices with high error rates whose effects can be reduced with circuit size. I spent the first month learning the features of the tket language in detail. During the first month, I also developed a script that translates tket into HQS' qoqo platform and vice versa. For the next two months, I focused on running experiments to test tket's optimization efficiency by compiling quantum simulation circuits. Such circuits represent the Trotterized time evolution and the fermionic swap network. In addition, I tested the compilation of large quantum simulation circuits for benchmarking. At the end of the internship, I gave a presentation about my work at the HQS seminar.

I applied to HQS because I wanted to work closely with the products in the field of quantum computing that can potentially accelerate the process of drug discovery.

Moreover, I was interested in learning more about the software side of the field. This internship met my expectations, since it not only equipped me with valuable skills but also helped me explore career opportunities in the field. This is thanks to the fact that my supervisor and everyone in the company was very approachable for questions and discussions. The main difference in comparison to the master thesis work is that I felt it is more fast-paced, due to the daily meetings where I had to inform the progress of my work. A tip for future applicants is to be comfortable with programming in python — there will be a coding assessment as part of the selection process as well.