Two-Month Visit to the Kageyama Group at Kyoto University

Linda Sophie Reitz (Prof. Richard Dronskowski Group)

Chair of Solid-State and Quantum Chemistry, Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany

Thanks to the funding by the Mixed-Anion ASPIRE program, I was given the opportunity to stay in the Kageyama group at Kyoto University for two months. My stay started in the middle of May and continued until the 15th of July 2025. As part of Univ.-Prof. Dronskowski's Group, my research focus lies in theoretical solid-state chemistry. More specifically, I focus on the development and implementation of new tools into the LOBSTER program package. Furthermore, I dedicate my time to crystal-structure prediction using evolutionary algorithms, in particular for small molecules at high pressure.

In this report I will describe how during this stay at Kyoto University I was not only able to get to know the group and Kyoto itself, but also how I was able to apply my knowledge to work on collaborative projects and teach about the LOBSTER program. Staying at the Kageyama group, I was able to gain insights into their work and expand my horizon regarding systems that I had not studied theoretically before. I met wonderful people who not only gave me insights into their work but also planned fun events. I was able to live in and explore beautiful Japan—an opportunity that I am extremely grateful for.

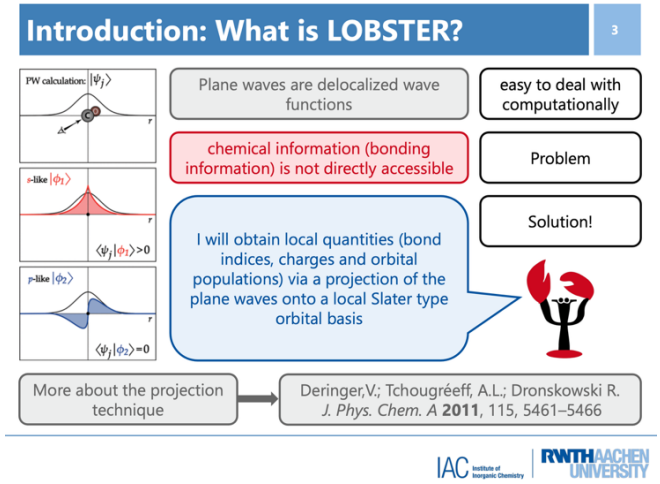

Fig. 1: What is LOBSTER? A slide from the lecture materials of the LOBSTER school explaining the thought behind

Research Objectives

Before I write about life and experiences in Kyoto, I will first introduce my objectives of this trip which developed to be two-fold. My first objective included the discussion of possible collaborations with the researchers from the Kageyama group. The second objective of my trip formed during the stay itself. The interest in using the LOBSTER program was quite high in the Kageyama group, which is why towards the end of my stay, I taught a two-day LOBSTER school for the interested group members.

Collaborative Projects Resulting from this Stay

The stay at the Kageyama lab was rather fruitful as regards collaborative projects. I was happy to show what theory can do and to get to know the group members face to face which will facilitate possible future collaborations.

For the first project, which has already advanced the most, I am very grateful to PhD student Artem Gabov.

He involved me in his project on an antiperovskite-related ternary subnitride early on during my stay. He approached me because he wanted to discuss the bonding in his system, more specifically the nature of the shortest metal–metal bond. Together we performed LOBSTER calculations and decided on using the crystal orbital bond index (COBI) to describe the bonding situation in his system. We chose this descriptor because the integrated value of the COBI (ICOBI) equals the bond order, making results easy to understand without having to look up reference values. By analyzing the Density of States (DOS) we were able to successfully identify the metallic character of the bond. All results have been implemented into a manuscript which is currently in writing.

Apart from this project, I had the opportunity to discuss with further group members. At the be-ginning of my stay Assoc. Prof. Tong Zhu approached me to gain insights into my work as well as to show me what he was working on, which was a great starting point for me in this group. I also discussed with students Shohei Kawanishi, Wenzheng Wu and Tatsuya Tsumori. I had multiple conversations with Assoc. Prof. Suguru Yoshida about his research, which will also result in a collaboration on an Indium compound and related systems.

Teaching a Two-Day LOBSTER School

As alluded to before, I noticed during my stay that there was a large interest in using the LOBSTER program. Many of the students already had some experience using density functional theory (DFT) codes e.g. VASP for structural optimization and some had already used LOBSTER before. After being approached by several students who wanted to learn more about the program, I decided to offer a LOBSTER school. This idea was met with support from Prof. Kageyama and I was grateful to get the opportunity to teach.

The school itself took place in the afternoon on June 3rd and continued in the morning on June 4th. The first day was reserved for the basic steps. These involved the preparation of LOBSTER calculations by first performing a VASP calculation to write out the wavefunctions. I quickly introduced the thought behind the LOBSTER program and what can be learned about a given system

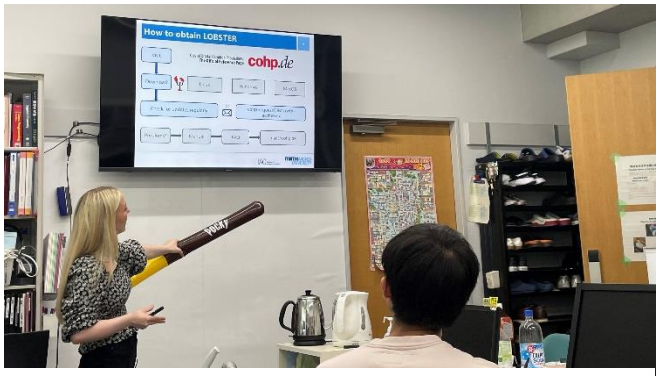

Fig. 2: Teaching a two-day LOBSTER school.
No Pocky required to become a LOBSTER expert!

even with basic input. Before school started, I had gained access to the group's cluster by the help of Assoc. Prof. Suguru Yoshida and had familiarized myself with their computational architecture. The group has a nicely set up internal cluster with six computational nodes. I had prepared examples on said cluster for every participant to try out the steps that we were going through in the school.

There were multiple breaks during the school for the participants to try what was just learned using the example systems on the cluster. During this time, I was thankful to be supported by Assoc. Prof. Suguru Yoshida and Asst. Prof. Daichi Kato who went around the room with me offering advice.

The second day of the school was reserved for the more advanced LOBSTER features. We mainly focused on the recently published fragment molecular orbitals (FMO) feature and talked about how to use it. Visualization and treatment of the results were also part of this day, and we worked on another example to get to know the feature better. After the school finished, I was delighted by the feedback from participants who used the FMO-feature right away.

Life and Experiences in Kyoto and Japan

Accommodation and Everyday Life

I was happy to be accommodated in the Marutamachi neighborhood close to the great Nijo-jo castle. The neighborhood was beautiful and full of high-quality cafes and restaurants as well as small art shops, which I loved to explore. In the evenings on my way back from university I often enjoyed a stroll through the beautifully lit streets in this part of the town.

On campus I was hosted in one of the main student offices which was perfect because it gave me the opportunity to experience life in the group and start conversations with other researchers more easily. On campus I also enjoyed the perks of the cafeteria with its restaurant-quality food. Lunches were organized many times with researchers from the group and Prof. Kageyama himself. Mondays were typically reserved for Kenso, the group's internal seminar. It was very interesting to attend because it allowed me to learn about the wide array of both experimental and theoretical research performed in the Kageyama group. I also had the opportunity to give a talk on my own research and was pleased by the resulting fruitful discussion.

Experiences in Kyoto and Japan

On the weekends, I managed to see a multitude of the beautiful sights that Kyoto itself has to offer e.g. the golden pavilion Kinkaku-ji, the silver pavilion Ginkaku-ji, the Kiyomizu-dera temple and towards the end even the start of the Gion festival. I also visited Osaka many times and did day trips to Kobe, Nara and Mount Hiei. I also visited Tokyo for a weekend and was quite impressed by this beautiful modern city.

There were also some places I would have never been able to visit without the great people that I met in the Kageyama group. I would especially like to thank Kei Morisato for taking me to the beautiful green tea producing area Wacuka and later on to Uji, where we tried a three-course meal of fresh green tea soba. We also visited the Byodoin temple that is displayed on the 10 ¥ coin and enjoyed refreshing matcha ice cream.

I am also very grateful to Assoc. Prof. Tong Zhu who invited us to an amazing traditional Chinese dinner where we were able to try very spicy dishes. It was a fun evening with delicious food and a great farewell. Assoc. Prof. Suguru Yoshida and Kay Morisato also made an effort to give us a nice farewell. They organised a fun evening at an Izakaya where we enjoyed great company, fun con-versations and a multiple-course meal specifically designed for our group.

Fig. 3: A lovely day in Uji with (from the left) Kayla Huang, Kei Morisato, Honoka Fukuda and Hicham

Final Remarks

I would like to express my gratitude to the ASPIRE program for allowing me to visit the Kageyama group at Kyoto University. I would like to thank Prof. Kageyama for generously hosting me and especially for the great conversations—both fun and productive—, discussions and advice that I got from him during my stay. I would like to thank him for being so supportive of me collaborating with his group members and for giving me the opportunity to teach about LOBSTER. My thanks also go to Prof. Dronskowski for recommending me and therefore giving me the opportunity to have this wonderful experience. I would like to thank all other Kageyama group members for the lovely time at Kyoto University. Thank you for the productive and memory-rich time in Japan!

Fig. 4: The last day at Kyoto University, saying goodbye to Prof. Kageyama.